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SPACE-GROUP SYMMETRY

Edited by

MOIS I. AROYO

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Foreword to the Sixth Edition

Standardizing the space-group tables has been a priority for crystallographers since at least 1929. The 1935 publication of the first set of such tables predated the founding of the International Union of Crystallography (IUCr) by 12 years. That book was one of the two volumes of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (or *International Tables for the Determination of Crystal Structures*). It established conventions so fundamental to the field that it is hard to imagine the confusion they prevented.

Major revisions of the space-group tables were published by the IUCr in 1952 (*International Tables for X-ray Crystallography* Volume I: *Symmetry Groups*) and 1983 (*International Tables for Crystallography* Volume A: *Space-Group Symmetry*). The considerably revised fifth edition of Volume A was made available online in 2006 at http://it.iucr.org/ along with the other seven volumes of the series as *International Tables Online*, which features many links within and between the electronic versions of the volumes. In 2011 the online series was complemented by the addition of the *Symmetry Database*, which provides more extensive symmetry information than do the volumes themselves.

Over the decades the information about space-group symmetry has been expanded so greatly that no single volume can contain it all. Some information about group–subgroup relationships was present in the 1935 volume but was left out of the 1952 edition. That information, augmented by some group–supergroup relationships, reappeared in the 1983 book. A full treatment of the subject was published in 2004 as the new Volume A1: *Symmetry Relations Between Space Groups*. The ability to follow electronic links back and forth between the online versions of Volumes A and A1 makes their combination very powerful.

In 2002 the new Volume E, *Subperiodic Groups*, was published. It contains the tables for the space groups of two-dimensional patterns that are periodic in only one dimension (the frieze groups) and three-dimensional patterns that are periodic in only one dimension (the rod groups) or two dimensions (the layer groups). The distinction between the 80 layer groups and the 17 plane groups is important. The latter had been included since 1952 along with the 230 space groups because the plane groups are so useful for teaching; they do not, however, allow for layer thickness. Layer groups may have more symmetry elements than are allowed for a plane group, *i.e.* inversion centers, a mirror plane within the layer, and 2 and 2_1 axes within the layer.

The new Volume C: *Mathematical, Physical and Chemical Tables* appeared in 1992 as a successor to Volume II of *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, which had grown to Volumes II–IV of the series *International Tables for X-ray Crystallography*; Volume C includes a section on the symmetry descriptions of commensurately and incommensurately modulated structures. Since then, that field has grown so much that the material is currently being expanded and relocated to the next edition of Volume B, *Reciprocal Space*.

Symmetry descriptions of magnetic structures are still under development. The number of magnetic groups is so large that any volume of *International Tables* listing them will have to be electronic only. In 2014, as an interim step, the IUCr published an e-book by D. B. Litvin (*Magnetic Group Tables*) that is available for downloading from the IUCr website at http://www.iucr.org/publ/978-0-9553602-2-0.

Because Volume A is usually the first volume of *International Tables* encountered by non-experts, an important aim of this edition has been to make its contents more accessible. The text sections have been completely reorganized and new introductory chapters have been written by authors experienced in teaching crystallography at all levels. Many explanatory examples have been added, and the terms and symbols used have been made consistent throughout. Diagrams for the cubic space groups have been redrawn so that they are easier to comprehend and axis labels have been added for the orthorhombic groups. Introductions to the topics covered in Volumes A1 and E, as well as to magnetic symmetry, have been added.

Volume A continues to evolve; this new edition, the sixth, is a major revision intended to meet the needs of scientists in the Electronic Age: users of the online version will also have access to the *Symmetry Database*, which is under continuous development and contains far more data than can be presented in print. The database can be used to calculate, among other things, the symmetry operations and Wyckoff positions for nonstandard settings in order to facilitate the tracking of symmetry relationships through a series of phase transitions or chemical substitutions.

We are all greatly indebted to Mois Aroyo, the Editor of this edition, for having had the vision for this revision of Volume A and for then having seen the project through. Getting experts to write for a wide group of readers and to agree on consistent terminology required erudition, tact and patience, all of which Mois has displayed in abundance.

Those who have been involved with this sixth edition are also indebted to all the crystallographers who contributed to previous editions. Two of the longtime architects of Volumes A and A1, Theo Hahn and Hans Wondratschek, recently passed on, but not before making very significant contributions towards the preparation of this new edition. It is an honor to acknowledge their many contributions.

Carolyn Pratt Brock
Editor-in-Chief, *International Tables for Crystallography*

Preface

Like its predecessors, this new sixth edition of *International Tables for Crystallography*, Volume A (referred to as *IT*A 6) treats the symmetries of two- and three-dimensional space groups and point groups in direct space. It is the reference work for crystal symmetry and provides standard symmetry data which are indispensable for any crystallographic or structural study. The text and data in *IT*A 6 fall into three main parts: Part 1 serves as a didactic introduction to space-group symmetry; Part 2 contains the authoritative tabulations of plane and space groups, and a guide to the tabulated data; and Part 3 features articles on more specialized, advanced topics.

Apart from new topics and developments, this sixth edition includes important modifications of the contents and of the arrangement of the text and the tabulated material of the previous (fifth) edition (*IT*A 5). The most salient feature of this edition is the introductory material in Part 1, which offers a homogeneous text of educational and teaching nature explaining the different kinds of symmetry information found in the tables. Although the first part is designed to provide a didactic introduction to symmetry in crystallography, suitable for advanced undergraduate and postgraduate students and for researchers from other fields, it is not meant to serve as an elementary textbook: readers are expected to have a basic understanding of the subject. The following aspects of symmetry theory are dealt with in Part 1:

Chapter 1.1 (Souvignier) offers a general introduction to group theory, which provides the mathematical background for considering symmetry properties. Starting from basic principles, those properties of groups are discussed that are of particular interest in crystallography. Essential topics like group–subgroup relationships, homomorphism and isomorphism, group actions and Wyckoff positions, conjugacy and equivalence relations or group normalizers are treated in detail and illustrated by crystallographic examples.

Chapter 1.2 (Wondratschek and Aroyo) deals with the types of crystallographic symmetry operations and the application of the matrix formalism in their description. The procedure for the geometric interpretation of a matrix–column pair of a symmetry operation is thoroughly explained and demonstrated by several instructive examples. The last section of the chapter provides a detailed discussion of the key concepts of a symmetry element and its constituents, a geometric element and an element set.

Chapter 1.3 (Souvignier) presents an introduction to the structure and classification of crystallographic space groups. Fundamental concepts related to translation lattices, such as the metric tensor, the unit cell and the distinction into primitive and centred lattices are rigorously defined. The action of point groups on translation lattices and the interplay between point groups and lattices is discussed in detail and, in particular, the distinction between symmorphic and non-symmorphic groups is explained. The final part of this chapter deals with various classification schemes of crystallographic space groups, including the classification into space-group types, geometric crystal classes and Bravais types of lattices.

Chapter 1.4 (Souvignier, Wondratschek, Aroyo, Chapuis and Glazer) handles various crystallographic terms used for the presentation of the symmetry data in the space-group tables. It starts with a detailed introduction to Hermann–Mauguin symbols for space, plane and crystallographic point groups, and to their Schoenflies symbols. A description is given of the symbols used for symmetry operations, and of their listings in the general-position and in the symmetry-operations blocks of the space-group tables. The Seitz notation for symmetry operations adopted by the Commission on Crystallographic Nomenclature as the standard convention for Seitz symbolism of the International Union of Crystallography [Glazer *et al.* (2014). *Acta Cryst.* A**70**, 300–302] is described and the Seitz symbols for the plane- and space-group symmetry operations are tabulated. The so-called additional symmetry operations of space groups resulting from the combination of the generating symmetry operations with lattice translations are introduced and illustrated. The classification of points in direct space into general and special Wyckoff positions, and the study of their site-symmetry groups and Wyckoff multiplicities are presented in detail. The final sections of the chapter offer a helpful introduction to two-dimensional sections and projections of space groups and their symmetry properties.

Chapter 1.5 (Wondratschek, Aroyo, Souvignier and Chapuis) introduces the mathematical tools necessary for performing coordinate transformations. The transformations of crystallographic data (point coordinates, space-group symmetry operations, metric tensors of direct and reciprocal space, indices of reflection conditions *etc*.) under a change of origin or a change of the basis are discussed and demonstrated by examples. More than 40 different types of coordinate-system transformations representing the most frequently encountered cases are listed and illustrated. Finally, synoptic tables of the space and plane groups show a large selection of alternative settings and their Hermann–Mauguin symbols covering most practical cases. It is worth pointing out that, in contrast to *IT*A 5, the extended Hermann–Mauguin symbols shown in the synoptic tables follow their original definition according to which the characters of the symbols indicate symmetry operations, and not symmetry elements.

Chapter 1.6 (Shmueli, Flack and Spence) offers a detailed presentation of methods of determining the symmetry of single-domain crystals from diffraction data, followed by a brief discussion of intensity statistics and their application to real intensity data from a $P\bar{1}$ crystal structure. The theoretical background for the derivation of the possible general reflections is introduced along with a brief discussion of special reflection conditions. An extensive tabulation of general reflection conditions and possible space groups is presented. The chapter concludes with a description and illustration of symmetry determination based on electron-diffraction methods, principally using convergent-beam electron diffraction.

Chapter 1.7 (Wondratschek, Müller, Litvin and Kopský) gives a short outline of the content of *International Tables for Crystallography* Volume A1, which is devoted to symmetry relations

between space groups, and also of the content of *International Tables for Crystallography* Volume E, in which two- and three-dimensional subperiodic groups are treated. The chapter starts with a brief introduction to the different kinds of maximal subgroups and minimal supergroups of space groups. The relations between the Wyckoff positions for group–subgroup-related space groups and their crystallographic applications are discussed. Illustrative examples of the application of the relationship between a crystal space group and the subperiodic-group symmetry of planes that transect the crystal in the determination of the layer-group symmetry of such planes and of domain walls are also given.

The essential data in Volume A are the diagrams and tables of the 17 types of plane groups and of the 230 types of space groups shown in Chapters 2.2 and 2.3 of Part 2. For each group type the following symmetry data are presented: a headline block with the relevant group symbols; diagrams of the symmetry elements and of the general positions; specifications of the origin and of the asymmetric unit; symmetry operations; generators; general and special Wyckoff positions with multiplicities, site symmetries, coordinate triplets and reflection conditions; and symmetries of special projections (for the space-group types). Compared to the tabulated symmetry data in *IT*A 5, two important differences are to be noted:

(i) The subgroups and supergroups of the space groups were listed as part of the space-group tables in the first to fifth editions of Volume A (from 1983 to 2005), but the listing was incomplete and lacked additional information on any basis transformations and origin shifts that may be involved. A complete listing of all maximal subgroups and minimal supergroups of all plane and space groups is now given in Volume A1 of *International Tables for Crystallography*, and to avoid repetition of the data tabulated there, the maximal-subgroup and minimal-supergroup data are omitted from the plane-group and space-group tables of *IT*A 6.

(ii) To improve the visualization and to aid interpretation of the complicated general-position diagrams of the cubic space groups, the stereodiagrams that were used for them in the previous editions of Volume A have been replaced by orthogonal-projection diagrams of the type given in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). In the new diagrams the points of the general position are shown as vertices of transparent polyhedra whose origins are chosen at special points of highest site symmetry. To provide a clearer three-dimensional style overview of the arrangements of the polyhedra, additional general-position diagrams in perspective projection are shown for each of the ten space groups of the $m\bar{3}m$ crystal class, and are included in a new four-page arrangement of the data for each of these space groups. The general-position diagrams of the cubic groups in both orthogonal and perspective projections were generated using the program *VESTA* [Momma & Izumi (2011). *J. Appl. Cryst.* **44**, 1272–1276].

There are further modifications of the symmetry data in the space-group tables, some of which deserve special mention:

(iii) To simplify the use of the symmetry-element diagrams for the three different projections of the orthorhombic space groups, the corresponding origins and basis vectors are explicitly labelled, as in the tables of the monoclinic space groups.

(iv) Modifications to the tabulated data and diagrams of the seven trigonal space groups of the rhombohedral lattice system (the so-called *rhombohedral* space groups) include: (*a*) changes in the sequence of coordinate triplets of some special Wyckoff positions of five rhombohedral groups [namely $R\bar{3}$ (148): Wyckoff positions 3*d* and 3*e*; $R32$ (155): 3*d* and 3*e*; $R3m$ (160): 3*b*; $R\bar{3}m$ (166): 3*d*, 3*e* and 6*h*; $R\bar{3}c$ (167): 6*d*] in the rhombohedral-axes settings in order to achieve correspondence between the sequences of coordinate triplets of the rhombohedral and hexagonal descriptions; (*b*) labelling of the basis vectors (cell edges) of the primitive rhombohedral cell in the general-position diagrams of the rhombohedral-axes setting descriptions of all rhombohedral space groups.

The diagrams and tables of the plane and space groups in Part 2 are preceded by a guide to their use, which includes lists of the symbols and terms used in them. In general, this guide (Chapter 2.1) follows the presentation of the material in *IT*A 5 but with several important exceptions related to the modifications of the content and the rearrangement of the material as discussed above. The improvements include new sections on: (i) symmetry elements (Hahn and Aroyo), explaining the important modifications of the tables of symbols of symmetry elements; (ii) Patterson symmetry (Flack), with tables of Patterson symmetries and symmetries of Patterson functions for all space and plane groups; and (iii) the general-position diagrams of the cubic groups (Momma and Aroyo). An extended section on the computer preparation of *IT*A 6 (Konstantinov and Momma) discusses the specific features of the computer programs and layout macros applied in the preparation of the set of diagrams and tables for this new edition.

Advanced and more specialized topics on space-group symmetry are treated in Part 3 of the volume. Most of the articles are substantially revised, upgraded and extended with respect to the versions in *IT*A 5. The major changes can be briefly described as follows:

In Chapter 3.1 on crystal lattices and their properties, the discussion of the Delaunay reduction procedure and the resulting classification of lattices into 24 Delaunay sorts (‘*Symmetrische Sorten*’) by Burzlaff and Zimmermann is supplemented by illustrative examples and a new table of data. Gruber and Grimmer broaden the description of conventional cells, showing that the conditions characterizing the conventional cells of the 14 Bravais types of lattices are only necessary and to make them sufficient they have to be extended to a more comprehensive system.

Chapter 3.2 on point groups and crystal classes (Hahn, Klapper, Müller and Aroyo) is substantially revised and new material has been added. The new developments include: (i) graphical presentations of the 47 face and point forms; (ii) enhancement of the tabulated Wyckoff-position data of the 10 two-dimensional and the 32 three-dimensional crystallographic point groups by the inclusion of explicit listings of the coordinate triplets of symmetry-equivalent points, and (iii) a new section on molecular symmetry (Müller), which treats noncrystallographic symmetries, the symmetry of polymeric molecules, and symmetry aspects of chiral molecules and crystal structures.

The revised text of Chapter 3.4 (Fischer and Koch) on lattice complexes is complemented by a thorough discussion of the concepts of orbit types, characteristic and non-characteristic orbits, and their comparison with the concepts of lattice complexes and limiting complexes.

Chapter 3.5 (Koch, Fischer and Müller) introduces and fully tabulates for the first time the chirality-preserving Euclidean normalizers of plane and space groups. Illustrative examples demonstrate the importance of the chirality-preserving Euclidean normalizers in the treatment of chiral crystal structures.

The new Chapter 3.6 (Litvin) on magnetic groups addresses the revival of interest in magnetic symmetry. The magnetic groups considered are the magnetic point groups, the two- and three-dimensional magnetic subperiodic groups, *i.e.* the magnetic frieze, rod and layer groups, and the one-, two- and three-dimensional magnetic space groups. After an introduction to magnetic symmetry groups, the existing nomenclatures for magnetic space groups are discussed and compared. The structure, symbols and properties of the magnetic groups and their maximal subgroups as listed in the electronic book by Litvin [*Magnetic Group Tables* (2014). IUCr: Chester. http://www.iucr.org/publ/978-0-9553602-2-0] are presented and illustrated.

Work on this sixth edition extended over the last eight years and many people have contributed to the successful completion of this complicated project. My acknowledgements should start with H. Wondratschek (Universität, Karlsruhe) and Th. Hahn (RWTH, Aachen), to whose memory this volume is dedicated. Their constant interest, support and sometimes hard but always constructive criticism were decisive during the preparation of this volume.

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Mois I. Aroyo
Editor, *International Tables for Crystallography* Volume A

Symbols for crystallographic items used in this volume

Direct space: points and vectors

$\mathbb{E}^n$	n-dimensional Euclidean point space
$\mathbb{V}^n$	n-dimensional vector space
$\mathbb{R}$, $\mathbb{Q}$, $\mathbb{Z}$	the field of real numbers, the field of rational numbers, the ring of integers
$\mathbf{L}$	lattice in $\mathbb{V}^3$
L	line in $\mathbb{E}^3$
$\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$; or $\mathbf{a}_i$	basis vectors of the lattice
a, b, c; or $\lvert\mathbf{a}\rvert$, $\lvert\mathbf{b}\rvert$, $\lvert\mathbf{c}\rvert$	lengths of basis vectors, lengths of cell edges (lattice parameters)
α, β, γ; or α_j	interaxial angles $\measuredangle(\mathbf{b}, \mathbf{c})$, $\measuredangle(\mathbf{c}, \mathbf{a})$, $\measuredangle(\mathbf{a}, \mathbf{b})$ (lattice parameters)
$\boldsymbol{G}$, g_{ik}	fundamental matrix (metric tensor) and its coefficients
V	cell volume
X, Y, Z, P	points
$\mathbf{r}$, $\mathbf{d}$, $\mathbf{x}$, $\mathbf{v}$, $\mathbf{u}$	vectors, position vectors
r, $\lvert\mathbf{r}\rvert$	norm, length of a vector
$\mathbf{x} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$	vector with coefficients x, y, z
x, y, z; or x_i	point coordinates expressed in units of a, b, c; coefficients of a vector
$\boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \equiv \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$	column of point coordinates or vector coefficients
$\mathbf{t}$	translation vector
t_1, t_2, t_3; or t_i	coefficients of translation vector $\mathbf{t}$
$\boldsymbol{t} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}$	column of coefficients of translation vector $\mathbf{t}$
O	origin
$\mathbf{o}$	zero vector (all coefficients zero)
$\boldsymbol{o}$	(3×1) column of zero coefficients
$\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$; or $\mathbf{a}'_i$	new basis vectors after a transformation of the coordinate system (basis transformation)
$\mathbf{r}'$; or $\mathbf{x}'$; x', y', z'; or x'_i	vector and point coordinates after a transformation of the coordinate system (basis transformation)
$\boldsymbol{x}' = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix}$	column of coordinates after a transformation of the coordinate system (basis transformation)
$\tilde{X}$	image of a point X after the action of a symmetry operation
$\tilde{x}$, $\tilde{y}$, $\tilde{z}$; or $\tilde{x}_i$	coordinates of an image point $\tilde{X}$
$\tilde{\boldsymbol{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix}$	column of coordinates of an image point $\tilde{X}$
$\mathbb{x}$, or $\mathbb{r}$	$(3 + 1) \times 1$ 'augmented' columns of point coordinates or vector coefficients

Directions and planes

$[uvw]$	indices of a lattice direction (zone axis)
$\langle uvw \rangle$	indices of a set of all symmetry-equivalent lattice directions
(hkl)	indices of a crystal face, or of a single net plane (Miller indices)
$(hkil)$	indices of a crystal face, or of a single net plane, for the hexagonal axes $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{c}$ (Bravais–Miller indices)
$\{hkl\}$	indices of a set of all symmetry-equivalent crystal faces ('crystal form'), or net planes
$\{hkil\}$	indices of a set of all symmetry-equivalent crystal faces ('crystal form'), or net planes, for the hexagonal axes $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, $\mathbf{c}$
hkl	indices of the Bragg reflection (Laue indices) from the set of parallel equidistant net planes (hkl)
d_{hkl}	interplanar distance, or spacing, of neighbouring net planes (hkl)

Reciprocal space

$\mathbf{L}^*$	reciprocal lattice
$\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$; or $\mathbf{a}_i^*$	basis vectors of the reciprocal lattice
a^*, b^*, c^*; or $\lvert\mathbf{a}^*\rvert$, $\lvert\mathbf{b}^*\rvert$, $\lvert\mathbf{c}^*\rvert$	lengths of basis vectors of the reciprocal lattice
α^*, β^*, γ^*; or α_j^*	interaxial angles $\measuredangle(\mathbf{b}^*, \mathbf{c}^*)$, $\measuredangle(\mathbf{c}^*, \mathbf{a}^*)$, $\measuredangle(\mathbf{a}^*, \mathbf{b}^*)$ of the reciprocal lattice
$\mathbf{r}^*$, or $\mathbf{h}$	vector in reciprocal space, or vector of reciprocal lattice
r^*, or $\lvert\mathbf{r}^*\rvert$	length of a vector in reciprocal space
h, k, l; or h_i	coefficients of a reciprocal-lattice vector
$\boldsymbol{h} = (h, k, l)$	(1×3) row of coefficients of a reciprocal-lattice vector
V^*	cell volume of the reciprocal lattice
$\boldsymbol{G}^*$, g_{ik}^*	fundamental matrix (metric tensor) of the reciprocal lattice and its coefficients

Functions

$\rho(xyz)$	electron density at the point x, y, z
$P(uvw)$	Patterson function for a vector with coefficients u, v, w
$F(hkl)$, or F	structure factor (of the unit cell) corresponding to the Bragg reflection hkl
$\lvert F(hkl)\rvert$, or $\lvert F\rvert$	modulus of the structure factor $F(hkl)$
$\alpha(hkl)$, or α	phase angle of the structure factor $F(hkl)$

Mappings, symmetry operations and their matrix–column presentation

$\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{W}$	(3 × 3) matrices describing the linear part of a mapping
A_{ik}, W_{ik}	matrix coefficients
$\boldsymbol{I}$	(3 × 3) unit matrix
$\boldsymbol{A}^{\mathrm{T}}$	matrix $\boldsymbol{A}$ transposed
$\det(\boldsymbol{A})$, $\mathrm{tr}(\boldsymbol{A})$	determinant of matrix $\boldsymbol{A}$, trace of matrix $\boldsymbol{A}$
$\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$	(3 × 1) column of coefficients w_i describing the translation part of a mapping
$\boldsymbol{w}_g$	intrinsic translation part of a symmetry operation
$\boldsymbol{w}_l$	location translation part of a symmetry operation
A, I, W	mappings, symmetry operations
t	translation symmetry operation
$(\boldsymbol{W}, \boldsymbol{w})$	matrix–column pair of a symmetry operation given by a (3 × 3) matrix $\boldsymbol{W}$ and a (3 × 1) column $\boldsymbol{w}$
$(\boldsymbol{I}, \boldsymbol{t})$	matrix–column pair of a translation
$(\boldsymbol{I}, \boldsymbol{o})$	matrix–column pair of the identity
$(\boldsymbol{P}, \boldsymbol{p})$	transformation of the coordinate system, described by a (3 × 3) matrix $\boldsymbol{P}$ and a (3 × 1) column $\boldsymbol{p}$
$(\boldsymbol{Q}, \boldsymbol{q})$	inverse transformation of $(\boldsymbol{P}, \boldsymbol{p})$: $(\boldsymbol{Q}, \boldsymbol{q}) = (\boldsymbol{P}, \boldsymbol{p})^{-1}$
$\mathbb{W}$	symmetry operation W, described by a (3 + 1) × (3 + 1) 'augmented' matrix
$\mathbb{P}$	transformation of the coordinate system, described by a (3 + 1) × (3 + 1) 'augmented' matrix
$\mathbb{Q}$	inverse transformation of $\mathbb{P}$: $\mathbb{Q} = \mathbb{P}^{-1}$
$\{\boldsymbol{R}\|\boldsymbol{v}\}$	Seitz symbol of a symmetry operation

Groups

$\mathcal{G}$	group, space group
$\mathcal{H}, \mathcal{U}$	subgroups
$\mathcal{I}$	trivial group, consisting of the unit element e only
$\mathcal{P}, \mathcal{S}, \mathcal{F}, \mathcal{D}, \mathcal{R}$	groups
$\|\mathcal{G}\|$	order of the group $\mathcal{G}$
i, or $[i]$	index of a subgroup in a group
$\mathcal{T}$, or $\mathcal{T}_\mathcal{G}$	group of all translations of a space group, or of the space group $\mathcal{G}$
$\mathcal{P}$, or $\mathcal{P}_\mathcal{G}$	point group of a space group, or of the space group $\mathcal{G}$
$\mathcal{M}$	Hermann's group
$\mathcal{A}$	group of all affine mappings (affine group)
$\mathcal{E}$	group of all isometries (motions) (Euclidean group)
$\mathcal{E}^+$	group of chirality-preserving isometries
φ, $ker(\varphi)$	homomorphic mapping (homomorphism), kernel of homomorphism φ
$\mathcal{G}/\mathcal{H}$	factor group or quotient group of $\mathcal{G}$ by $\mathcal{H}$
$\mathcal{N}_\mathcal{G}(\mathcal{H})$	normalizer of $\mathcal{H}$ in $\mathcal{G}$
$\mathcal{N}_\mathcal{E}(\mathcal{G})$, or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$	Euclidean or chirality-preserving Euclidean normalizer of the space group $\mathcal{G}$
$\mathcal{N}_\mathcal{A}(\mathcal{G})$	affine normalizer of $\mathcal{G}$
$\mathcal{G}(\omega)$	orbit of ω under the group $\mathcal{G}$
$\mathcal{S}_\mathcal{G}(\omega)$, $\mathcal{S}_\mathcal{H}(\omega)$	stabilizer of ω in the group $\mathcal{G}$, or $\mathcal{H}$
$\mathcal{O} = \mathcal{G}(X)$	orbit of point X under the group $\mathcal{G}$
$\mathcal{S}_X = \mathcal{S}_\mathcal{G}(X)$	site-symmetry group of point X
$\mathscr{E}$	eigensymmetry group of an orbit $\mathcal{O}$
a, b, g, h, m, t	group elements
e	unit element of a group
t	element of the translation group $\mathcal{T}$

1.1. A general introduction to groups

B. Souvignier

In this chapter we give a general introduction to group theory, which provides the mathematical background for considering symmetry properties. Starting from basic principles, we discuss those properties of groups that are of particular interest in crystallography. To readers interested in a more elaborate treatment of the theoretical background, the standard textbooks by Armstrong (2010), Hill (1999) or Sternberg (2008) are recommended; an account from the perspective of crystallography can also be found in Müller (2013).

1.1.1. Introduction

Crystal structures may be investigated and classified according to their symmetry properties. But in a strict sense, crystal structures in nature are never perfectly symmetric, due to impurities, structural imperfections and especially their finite extent. Therefore, symmetry considerations deal with *idealized* crystal structures that are free from impurities and structural imperfections and that extend infinitely in all directions. In the mathematical model of such an idealized crystal structure, the atoms are replaced by points in a three-dimensional point space and this model will be called a *crystal pattern*.

A symmetry operation of a crystal pattern is a transformation of three-dimensional space that preserves distances and angles and that leaves the crystal pattern as a whole unchanged. The symmetry of a crystal pattern is then understood as the collection of all symmetry operations of the pattern.

The following simple statements about the symmetry operations of a crystal pattern are almost self-evident:

(*a*) If two symmetry operations are applied successively, the crystal pattern is still invariant, thus the combination of the two operations (called their *composition*) is again a symmetry operation.

(*b*) Every symmetry operation can be reversed by simply moving every point back to its original position.

These observations (together with the fact that leaving all points in their position is also a symmetry operation) show that the symmetry operations of a crystal pattern form an algebraic structure called a *group*.

1.1.2. Basic properties of groups

Although groups occur in innumerable contexts, their basic properties are very simple and are captured by the following definition.

Definition. Let $\mathcal{G}$ be a set of elements on which a binary operation is defined which assigns to each pair (g, h) of elements the composition $g \circ h \in \mathcal{G}$. Then $\mathcal{G}$, together with the binary operation $\circ$, is called a *group* if the following hold:

(i) the binary operation is associative, *i.e.* $(g \circ h) \circ k = g \circ (h \circ k)$;

(ii) there exists a *unit element* or *identity element* $e \in \mathcal{G}$ such that $g \circ e = g$ and $e \circ g = g$ for all $g \in \mathcal{G}$;

(iii) every $g \in \mathcal{G}$ has an inverse element, denoted by g^{-1}, for which $g \circ g^{-1} = g^{-1} \circ g = e$.

In most cases, the composition of group elements is regarded as a *product* and is written as $g \cdot h$ or even gh instead of $g \circ h$. An exception is groups where the composition is addition, *e.g.* a group of translations. In such a case, the composition $\mathbf{a} \circ \mathbf{b}$ is more conveniently written as $\mathbf{a} + \mathbf{b}$.

Examples

(i) The group consisting only of the identity element e (with $e \circ e = e$) is called the *trivial group*.

(ii) The group $3m$ of all symmetries of an equilateral triangle is a group with the composition of symmetry operations as binary operation. The group contains six elements, namely three reflections, two rotations and the identity element. It is schematically displayed in Fig. 1.1.2.2.

(iii) The set $\mathbb{Z}$ of all integers forms a group with addition as operation. The identity element is 0, the inverse element for $a \in \mathbb{Z}$ is $-a$.

(iv) The set of complex numbers with absolute value 1 forms a circle in the complex plane, the *unit circle* S^1. The unit circle can be described by $S^1 = \{\exp(2\pi i\, t) \mid 0 \leq t < 1\}$ and forms a group with (complex) multiplication as operation.

(v) The set of all real $n \times n$ matrices with determinant $\neq 0$ is a group with matrix multiplication as operation. This group is called the *general linear group* and denoted by $\mathrm{GL}_n(\mathbb{R})$.

If a group $\mathcal{G}$ contains finitely many elements, it is called a *finite group* and the number of its elements is called the *order* of the group, denoted by $|\mathcal{G}|$. A group with infinitely many elements is called an *infinite group*.

For a group element g, its *order* is the smallest integer $n > 0$ such that $g^n = e$ is the identity element. If there is no such integer, then g is said to be of *infinite order*.

The group operation is not required to be *commutative*, *i.e.* in general one will have $gh \neq hg$. However, a group $\mathcal{G}$ in which $gh = hg$ for all g, h is said to be a *commutative* or *abelian group*.

The inverse of the product gh of two group elements is the product of the inverses of the two elements in reversed order, *i.e.* $(gh)^{-1} = h^{-1}g^{-1}$.

A particularly simple type of groups is *cyclic groups* in which all elements are powers of a single element g. A finite cyclic group $\mathcal{C}_n$ of order n can be written as $\mathcal{C}_n = \{g, g^2, \ldots, g^{n-1}, g^n = e\}$. For example, the rotations that are symmetry operations of an equilateral triangle constitute a cyclic group of order 3.

The group $\mathbb{Z}$ of integers (with addition as operation) is an example of an infinite cyclic group in which negative powers also have to be considered, *i.e.* where $\mathcal{G} = \{\ldots, g^{-2}, g^{-1}, e = g^0, g^1, g^2, \ldots\}$.

Groups of small order may be displayed by their *multiplication table*, which is a square table with rows and columns indexed by the group elements and where the intersection of the row labelled by g and of the column labelled by h is the product gh. It follows immediately from the invertibility of the group elements that each row and column of the multiplication table contains every group element precisely once.

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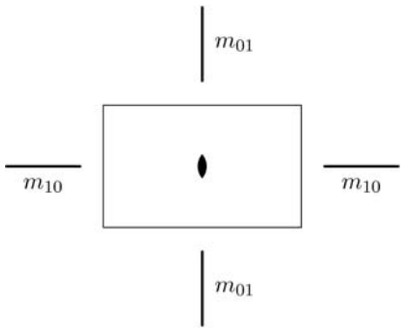

Figure 1.1.2.1
Symmetry group 2*mm* of a rectangle.

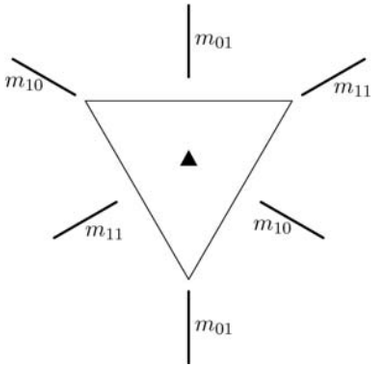

Figure 1.1.2.2
Symmetry group 3*m* of an equilateral triangle.

Examples

(i) A cyclic group of order 3 consists of the elements $\{g, g^2, g^3 = e\}$. Its multiplication table is

	e	g	g^2
e	e	g	g^2
g	g	g^2	e
g^2	g^2	e	g

(ii) The symmetry group 2*mm* of a rectangle (with unequal sides) consists of a twofold rotation 2, two reflections m_{10}, m_{01} with mirror lines along the coordinate axes and the identity element 1 (see Fig. 1.1.2.1; the small black lenticular symbol in the centre represents the twofold rotation point).
Note that in this and all subsequent examples of crystallographic point groups we will use the Seitz symbols (*cf.* Section 1.4.2.2) for the symmetry operations and the Hermann–Mauguin symbols (*cf.* Section 1.4.1) for the point groups.
The multiplication table of the group 2*mm* is

	1	2	m_{10}	m_{01}
1	1	2	m_{10}	m_{01}
2	2	1	m_{01}	m_{10}
m_{10}	m_{10}	m_{01}	1	2
m_{01}	m_{01}	m_{10}	2	1

The symmetry of the multiplication table (with respect to the main diagonal) shows that this is an abelian group.

(iii) The symmetry group 3*m* of an equilateral triangle consists (apart from the identity element 1) of the threefold rotations 3^+ and 3^- and the reflections m_{10}, m_{01}, m_{11} with mirror lines through a corner of the triangle and the centre of the opposite side (see Fig. 1.1.2.2; the small black triangle in the centre represents the threefold rotation point).
The multiplication table of the group 3*m* is

	1	3^+	3^-	m_{10}	m_{01}	m_{11}
1	1	3^+	3^-	m_{10}	m_{01}	m_{11}
3^+	3^+	3^-	1	m_{11}	m_{10}	m_{01}
3^-	3^-	1	3^+	m_{01}	m_{11}	m_{10}
m_{10}	m_{10}	m_{01}	m_{11}	1	3^+	3^-
m_{01}	m_{01}	m_{11}	m_{10}	3^-	1	3^+
m_{11}	m_{11}	m_{10}	m_{01}	3^+	3^-	1

The fact that $3^+ \cdot m_{10} = m_{11}$, but $m_{10} \cdot 3^+ = m_{01}$ shows that this group is not abelian. It is actually the smallest group (in terms of order) that is not abelian.

(iv) The symmetry group 4*mm* of the square consists of the cyclic group generated by the fourfold rotation 4^+ containing the elements $1, 4^+, 2, 4^-$ and the reflections m_{10}, m_{01}, m_{11}, $m_{1\bar{1}}$ with mirror lines along the coordinate axes and the diagonals of the square (see Fig. 1.1.2.3; the small black square in the centre represents the fourfold rotation point).
The multiplication table of the group 4*mm* is

	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
1	1	2	4^+	4^-	m_{10}	m_{01}	m_{11}	$m_{1\bar{1}}$
2	2	1	4^-	4^+	m_{01}	m_{10}	$m_{1\bar{1}}$	m_{11}
4^+	4^+	4^-	2	1	m_{11}	$m_{1\bar{1}}$	m_{01}	m_{10}
4^-	4^-	4^+	1	2	$m_{1\bar{1}}$	m_{11}	m_{10}	m_{01}
m_{10}	m_{10}	m_{01}	$m_{1\bar{1}}$	m_{11}	1	2	4^-	4^+
m_{01}	m_{01}	m_{10}	m_{11}	$m_{1\bar{1}}$	2	1	4^+	4^-
m_{11}	m_{11}	$m_{1\bar{1}}$	m_{10}	m_{01}	4^+	4^-	1	2
$m_{1\bar{1}}$	$m_{1\bar{1}}$	m_{11}	m_{01}	m_{10}	4^-	4^+	2	1

This group is not abelian, because for example $4^+ \cdot m_{10} = m_{11}$, but $m_{10} \cdot 4^+ = m_{1\bar{1}}$.

The groups that are considered in crystallography do not consist of abstract elements but of symmetry operations with a geometric meaning. In the figures illustrating the groups and also in the symbols used for the group elements, this geometric nature is taken into account. For example, the fourfold rotation 4^+ in the group 4*mm* is represented by the small black square placed at the rotation point and the reflection m_{10} by the line fixed by the reflection. To each crystallographic symmetry operation a *geometric element* is assigned which characterizes the type of the

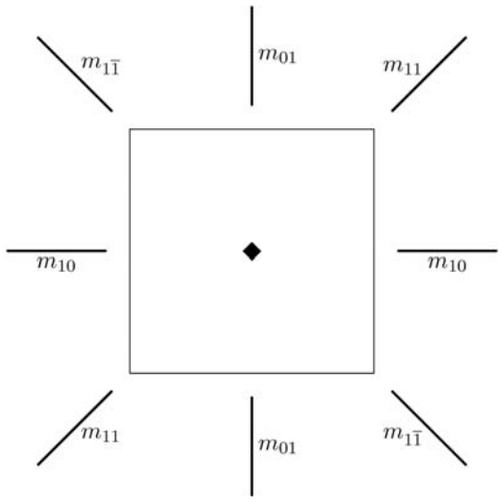

Figure 1.1.2.3
Symmetry group 4*mm* of the square.

symmetry operation. The precise definition of the geometric elements for the different types of operations is given in Section 1.2.3. For a rotation in three-dimensional space the geometric element is the line along the rotation axis and for a reflection it is the plane fixed by the reflection. Different symmetry operations may share the same geometric element, but these operations are then closely related, such as rotations around the same line. One therefore introduces the notion of a *symmetry element*, which is a geometric element together with its associated symmetry operations. In the figures for the crystallographic groups, the symbols like the little black square or the lines actually represent these symmetry elements (and not just a symmetry operation or a geometric element).

It is clear that for larger groups the multiplication table becomes unwieldy to set up and use. Fortunately, for many purposes a full list of all products in the group is actually not required. A very economic alternative of describing a group is to give only a small subset of the group elements from which all other elements can be obtained by forming products.

Definition. A subset $\mathcal{X} \subseteq \mathcal{G}$ is called a set of *generators* for $\mathcal{G}$ if every element of $\mathcal{G}$ can be obtained as a finite product of elements from $\mathcal{X}$ or their inverses. If $\mathcal{X}$ is a set of generators for $\mathcal{G}$, one writes $\mathcal{G} = \langle \mathcal{X} \rangle$.

A group which has a finite generating set is said to be *finitely generated*.

Examples

(i) Every finite group is finitely generated, since $\mathcal{X}$ is allowed to consist of all group elements.

(ii) A cyclic group is generated by a single element. In particular, the infinite cyclic group $(\mathbb{Z}, +)$ is generated by $\mathcal{X} = \{1\}$, but also by $\mathcal{X} = \{-1\}$.

(iii) The symmetry group $4mm$ of the square is generated by a fourfold rotation and any of the reflections, *e.g.* by $\{4^+, m_{10}\}$, but also by two reflections with reflection lines which are not perpendicular, *e.g.* by $\{m_{10}, m_{11}\}$.

(iv) The full symmetry group $m\bar{3}m$ of the cube consists of 48 elements. It can be generated by a fourfold rotation 4^+_{100} around the a axis, a threefold rotation 3^+_{111} around a space diagonal and the inversion $\bar{1}$. It is also possible to generate the group by only two elements, *e.g.* by the fourfold rotation 4^+_{100} and a reflection m_{110} in a plane with normal vector along one of the face diagonals of the cube.

(v) The additive group $(\mathbb{Q}, +)$ of the rational numbers is not finitely generated, because finite sums of finitely many generators $a_1/b_1, a_2/b_2, \ldots, a_n/b_n$ have denominators dividing $b_1 \cdot b_2 \cdot \ldots \cdot b_n$ and thus $1/(1 + b_1 \cdot b_2 \cdot \ldots \cdot b_n)$ is not a finite sum of these generators.

Although one usually chooses generating sets with as few elements as possible, it is sometimes convenient to actually include some redundancy. For example, it may be useful to generate the symmetry group $4mm$ of the square by $\{2, m_{10}, m_{11}\}$. The element 2 is redundant, since $2 = (m_{10}m_{11})^2$, but this generating set explicitly shows the different types of elements of order 2 in the group.

1.1.3. Subgroups

The group of symmetry operations of a crystal pattern may alter if the crystal undergoes a phase transition. Often, some symmetries are preserved, while others are lost, *i.e.* symmetry breaking takes place. The symmetry operations that are preserved form a subset of the original symmetry group which is itself a group. This gives rise to the concept of a subgroup.

Definition. A subset $\mathcal{H} \subseteq \mathcal{G}$ is called a *subgroup* of $\mathcal{G}$ if its elements form a group by themselves. This is denoted by $\mathcal{H} \leq \mathcal{G}$. If $\mathcal{H}$ is a subgroup of $\mathcal{G}$, then $\mathcal{G}$ is called a *supergroup* of $\mathcal{H}$. In order to be a subgroup, $\mathcal{H}$ is required to contain the identity element e of $\mathcal{G}$, to contain inverse elements and to be closed with respect to composition of elements. Thus, technically, every group is a subgroup of itself.

The subgroups of $\mathcal{G}$ that are not equal to $\mathcal{G}$ are called *proper subgroups* of $\mathcal{G}$. A proper subgroup $\mathcal{H}$ of $\mathcal{G}$ is called a *maximal subgroup* if it is not a proper subgroup of any proper subgroup $\mathcal{H}'$ of $\mathcal{G}$.

It is often convenient to specify a subgroup $\mathcal{H}$ of $\mathcal{G}$ by a set $\{h_1, \ldots, h_s\}$ of generators. This is denoted by $\mathcal{H} = \langle h_1, \ldots, h_s \rangle$. The order of $\mathcal{H}$ is not *a priori* obvious from the set of generators. For example, in the symmetry group $4mm$ of the square the pairs $\{m_{10}, m_{01}\}$ and $\{m_{11}, m_{1\bar{1}}\}$ both generate subgroups of order 4, whereas the pair $\{m_{10}, m_{11}\}$ generates the full group of order 8.

The subgroups of a group can be visualized in a *subgroup diagram*. In such a diagram the subgroups are arranged with subgroups of higher order above subgroups of lower order. Two subgroups are connected by a line if one is a maximal subgroup of the other. By following downward paths in this diagram, all group–subgroup relations in a group can be derived. Additional information is provided by connecting subgroups of the same order by a horizontal line if they are *conjugate* (see Section 1.1.7).

Examples

(i) The set $\{e\}$ consisting only of the identity element of $\mathcal{G}$ is a subgroup, called the *trivial subgroup* of $\mathcal{G}$.

(ii) For the group $\mathbb{Z}$ of the integers, all subgroups are cyclic and generated by some integer n, *i.e.* they are of the form $n\mathbb{Z} := \{na \mid a \in \mathbb{Z}\}$ for an integer n. Such a subgroup is maximal if n is a prime number.

(iii) For every element g of a group $\mathcal{G}$, the powers of g form a subgroup of $\mathcal{G}$ which is a cyclic group.

(iv) In $\mathrm{GL}_n(\mathbb{R})$ the matrices of determinant 1 form a subgroup, since the determinant of the matrix product $\boldsymbol{A} \cdot \boldsymbol{B}$ is equal to the product of the determinants of $\boldsymbol{A}$ and $\boldsymbol{B}$.

(v) In the symmetry group $3m$ of an equilateral triangle the rotations form a subgroup of order 3 (see Fig. 1.1.3.1).

(vi) The symmetry group $2mm$ of a rectangle has three subgroups of order 2, generated by the reflection m_{10}, the twofold rotation 2 and the reflection m_{01}, respectively (see Fig. 1.1.3.2).

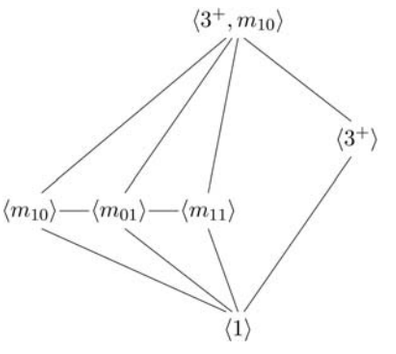

Figure 1.1.3.1
Subgroup diagram for the symmetry group $3m$ of an equilateral triangle.

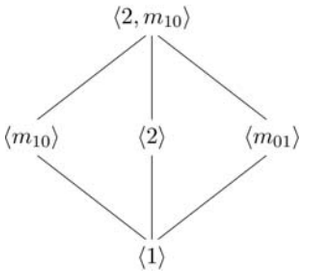

Figure 1.1.3.2
Subgroup diagram for the symmetry group 2*mm* of a rectangle.

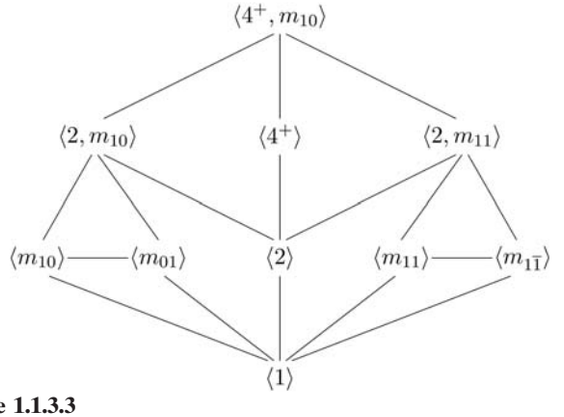

Figure 1.1.3.3
Subgroup diagram for the symmetry group 4*mm* of the square.

(vii) In the symmetry group 4*mm* of the square, the reflections m_{10} and m_{01} together with their product 2 and the identity element 1 form a subgroup of order 4. This subgroup can be recognized in the subgroup diagram of 4*mm* as the subdiagram of the subgroups of $\langle 2, m_{10}\rangle$ in the left part of Fig. 1.1.3.3 which coincides with the subgroup diagram of 2*mm* in Fig. 1.1.3.2. A different subgroup of order 4 is formed by the other pair of perpendicular reflections m_{11}, $m_{1\bar{1}}$ together with 2 and 1 and a third subgroup of order 4 is the cyclic subgroup $\langle 4^+\rangle$ generated by the fourfold rotation (see Fig. 1.1.3.3).

1.1.4. Cosets

A subgroup allows us to partition a group into disjoint subsets of the same size, called *cosets*.

Definition. Let $\mathcal{H} = \{h_1, h_2, h_3, \ldots\}$ be a subgroup of $\mathcal{G}$. Then for $g \in \mathcal{G}$ the set

$$g\mathcal{H} := \{gh_1, gh_2, gh_3, \ldots\} = \{gh \mid h \in \mathcal{H}\}$$

is called the *left coset* of $\mathcal{H}$ with *representative* g. Analogously, the *right coset* with representative g is defined as

$$\mathcal{H}g := \{h_1 g, h_2 g, h_3 g, \ldots\} = \{hg \mid h \in \mathcal{H}\}.$$

The coset $e\mathcal{H} = \mathcal{H} = \mathcal{H}e$ is called the *trivial coset* of $\mathcal{H}$.

Remarks

(i) Since two elements gh and gh' in the same coset $g\mathcal{H}$ can only be the same if $h = h'$, the elements of $g\mathcal{H}$ are in one-to-one correspondence with the elements of $\mathcal{H}$. In particular, for a finite subgroup $\mathcal{H}$ the number of elements in each coset of $\mathcal{H}$ equals the order $|\mathcal{H}|$ of the subgroup $\mathcal{H}$.

(ii) Every element contained in $g\mathcal{H}$ may serve as representative for this coset, *i.e.* $g'\mathcal{H} = g\mathcal{H}$ for every $g' \in g\mathcal{H}$. In particular, if an element g'' is contained in the intersection $g\mathcal{H} \cap g'\mathcal{H}$ of two cosets, one has $g''\mathcal{H} = g\mathcal{H}$ and $g''\mathcal{H} = g'\mathcal{H}$. This implies that two cosets are either disjoint (*i.e.* contain no common element) or they are equal.

These two remarks have an important consequence: since an element $g \in \mathcal{G}$ is contained in the coset $g\mathcal{H}$, the cosets of $\mathcal{H}$ partition the elements of $\mathcal{G}$ into sets of the same cardinality as $\mathcal{H}$ (which is of the order of $\mathcal{H}$ in the case where this is finite).

Definition. If the number of different cosets of a subgroup $\mathcal{H} \leq \mathcal{G}$ is finite, this number is called the *index* of $\mathcal{H}$ in $\mathcal{G}$, denoted by $[i]$ or $[\mathcal{G} : \mathcal{H}]$. Otherwise, $\mathcal{H}$ is said to have *infinite index* in $\mathcal{G}$.

In the case of a finite group, the partitioning of the elements of $\mathcal{G}$ into the cosets of $\mathcal{H}$ shows that both the order of $\mathcal{H}$ and the index of $\mathcal{H}$ in $\mathcal{G}$ divide the order of $\mathcal{G}$. This is summarized in the following famous result.

Lagrange's theorem

For a finite group $\mathcal{G}$ and a subgroup $\mathcal{H}$ of $\mathcal{G}$ one has

$$|\mathcal{G}| = |\mathcal{H}| \cdot [\mathcal{G} : \mathcal{H}],$$

i.e. the order of a subgroup multiplied by its index gives the order of the full group.

For example, a group of order n cannot have a proper subgroup of order larger than $n/2$.

Whether or not two cosets of a subgroup $\mathcal{H}$ are equal depends on whether the quotient of their representatives is contained in $\mathcal{H}$: for left cosets one has $g\mathcal{H} = g'\mathcal{H}$ if and only if $g^{-1}g' \in \mathcal{H}$ and for right cosets $\mathcal{H}g = \mathcal{H}g'$ if and only if $g'g^{-1} \in \mathcal{H}$.

Definition. If $\mathcal{H}$ is a subgroup of $\mathcal{G}$ and $g_1, g_2, g_3, \ldots \in \mathcal{G}$ are such that $g_i\mathcal{H} \neq g_j\mathcal{H}$ for $i \neq j$, and every $g \in \mathcal{G}$ is contained in some left coset $g_i\mathcal{H}$, then $g_1, g_2, g_3, \ldots$ is called a system of *left coset representatives* of $\mathcal{G}$ relative to $\mathcal{H}$. It is customary to choose $g_1 = e$ so that the coset $g_1\mathcal{H} = e\mathcal{H} = \mathcal{H}$ is the subgroup $\mathcal{H}$ itself. The decomposition

$$\mathcal{G} = \mathcal{H} \cup g_2\mathcal{H} \cup g_3\mathcal{H} \ldots$$

is called the *coset decomposition* of $\mathcal{G}$ into left cosets relative to $\mathcal{H}$.

Analogously, $g_1', g_2', g_3', \ldots \in \mathcal{G}$ is called a system of *right coset representatives* if $\mathcal{H}g_i' \neq \mathcal{H}g_j'$ for $i \neq j$ and every $g \in \mathcal{G}$ is contained in some right coset $\mathcal{H}g_i$. Again, one usually chooses $g_1' = e$ and the decomposition

$$\mathcal{G} = \mathcal{H} \cup \mathcal{H}g_2' \cup \mathcal{H}g_3' \ldots$$

is called the *coset decomposition* of $\mathcal{G}$ into right cosets relative to $\mathcal{H}$.

To obtain the coset decomposition one starts by choosing $\mathcal{H}$ as the first coset (with representative e). Next, an element $g_2 \in \mathcal{G}$ with $g_2 \notin \mathcal{H}$ is selected as representative for the second coset $g_2\mathcal{H}$. For the third coset, an element $g_3 \in \mathcal{G}$ with $g_3 \notin \mathcal{H}$ and $g_3 \notin g_2\mathcal{H}$ is required. If at a certain stage the cosets $\mathcal{H}, g_2\mathcal{H}, \ldots, g_m\mathcal{H}$ have been defined but do not yet exhaust $\mathcal{G}$, an element g_{m+1} not contained in the union $\mathcal{H} \cup g_2\mathcal{H} \cup \ldots \cup g_m\mathcal{H}$ is chosen as representative for the next coset.

Examples

(i) Let $\mathcal{G} = 3m$ be the symmetry group of an equilateral triangle and $\mathcal{H} = \langle 3^+\rangle$ its subgroup containing the rotations. Then for every reflection $m \in \mathcal{G}$ the elements e, m form a system of coset representatives of $\mathcal{G}$ relative to $\mathcal{H}$ and the coset decomposition is $\mathcal{G} = \{1, 3^+, 3^-\} \cup \{m_{10}, m_{01}, m_{11}\}$.

(ii) For any integer n, the set $n\mathbb{Z} := \{na \mid a \in \mathbb{Z}\}$ of multiples of n forms an infinite subgroup of index n in $\mathbb{Z}$. A system of coset representatives of $\mathbb{Z}$ relative to $n\mathbb{Z}$ is formed by the numbers $0, 1, 2, \ldots, n-1$. The coset with representative 0 is $\{\ldots, -n, 0, n, 2n, \ldots\}$, the coset with representative 1 is $\{\ldots, -n+1, 1, n+1, 2n+1, \ldots\}$ and an integer a belongs to the coset with representative k if and only if a gives remainder k upon division by n.

1.1.5. Normal subgroups, factor groups

In general, the left and right cosets of a subgroup $\mathcal{H}$ differ, for example in the symmetry group $3m$ of an equilateral triangle the left coset decomposition with respect to the subgroup $\mathcal{H} = \{1, m_{10}\}$ is

$$\begin{aligned}&\{1, m_{10}\} \cup 3^+\{1, m_{10}\} \cup 3^-\{1, m_{10}\}\\ =&\{1, m_{10}\} \cup \{3^+, m_{11}\} \cup \{3^-, m_{01}\},\end{aligned}$$

whereas the right coset decomposition is

$$\begin{aligned}&\{1, m_{10}\} \cup \{1, m_{10}\}3^+ \cup \{1, m_{10}\}3^-\\ =&\{1, m_{10}\} \cup \{3^+, m_{01}\} \cup \{3^-, m_{11}\}.\end{aligned}$$

For particular subgroups, however, it turns out that the left and right cosets coincide, *i.e.* one has $g\mathcal{H} = \mathcal{H}g$ for all $g \in \mathcal{G}$. This means that for every $h \in \mathcal{H}$ and every $g \in \mathcal{G}$ the element gh is of the form $gh = h'g$ for some $h' \in \mathcal{H}$ and thus $ghg^{-1} = h' \in \mathcal{H}$. The element $h' = ghg^{-1}$ is called the *conjugate of h by g*. Note that in the definition of the conjugate element there is a choice whether the inverse element g^{-1} is placed to the left or right of h. Depending on the applications that are envisaged and on the preferences of the author, both versions ghg^{-1} and $g^{-1}hg$ are found in the literature, but in the context of crystallographic groups it is more convenient to have the inverse g^{-1} to the right of h.

An important aspect of conjugate elements is that they share many properties, such as the order or the type of symmetry operation. As a consequence, conjugate symmetry operations have the same type of geometric elements. For example, if h is a threefold rotation in three-dimensional space, its geometric element is the line along the rotation axis. The geometric element of a conjugate element ghg^{-1} is then also a line fixed by a threefold rotation, but in general this line has a different direction.

Definition. A subgroup $\mathcal{H}$ of $\mathcal{G}$ is called a *normal subgroup* if $ghg^{-1} \in \mathcal{H}$ for all $g \in \mathcal{G}$ and all $h \in \mathcal{H}$. This is denoted by $\mathcal{H} \trianglelefteq \mathcal{G}$. For a normal subgroup $\mathcal{H}$, the left and right cosets of $\mathcal{G}$ with respect to $\mathcal{H}$ coincide.

Remarks

(i) The full group $\mathcal{G}$ and the trivial subgroup $\{e\}$ are always normal subgroups of $\mathcal{G}$. These are often called the *trivial* normal subgroups of $\mathcal{G}$.

(ii) In abelian groups, every subgroup is a normal subgroup, because $gh = hg$ implies $ghg^{-1} = h \in \mathcal{H}$.

(iii) A subgroup $\mathcal{H}$ of index 2 in $\mathcal{G}$ is always a normal subgroup, since the coset decomposition relative to $\mathcal{H}$ consists of only two cosets and for any element $g \notin \mathcal{H}$ the left and right cosets $g\mathcal{H}$ and $\mathcal{H}g$ both consist precisely of those elements of $\mathcal{G}$ that are not contained in $\mathcal{H}$. Therefore, $g\mathcal{H} = \mathcal{H}g$ for $g \notin \mathcal{H}$ and for $h \in \mathcal{H}$ clearly $h\mathcal{H} = \mathcal{H} = \mathcal{H}h$ holds.

(iv) In order to check whether a subgroup $\mathcal{H}$ of $\mathcal{G}$ is a normal subgroup it is sufficient to check whether $ghg^{-1} \in \mathcal{H}$ for generators g of $\mathcal{G}$ and generators h of $\mathcal{H}$. This is due to the fact that on the one hand $(g_1g_2)\,h\,(g_1g_2)^{-1} = g_1(g_2hg_2^{-1})g_1^{-1}$ and on the other hand $g(h_1h_2)g^{-1} = (gh_1g^{-1})(gh_2g^{-1})$.

Examples

(i) In the symmetry group $3m$ of an equilateral triangle, the subgroup generated by the threefold rotation 3^+ is a normal subgroup because it is of index 2 in $3m$.
The subgroups of order 2 generated by the reflections m_{10}, m_{01} and m_{11} are not normal because $3^+ \cdot m_{10} \cdot 3^- = m_{01} \notin \langle m_{10}\rangle$, $3^+ \cdot m_{01} \cdot 3^- = m_{11} \notin \langle m_{01}\rangle$ and $3^+ \cdot m_{11} \cdot 3^- = m_{10} \notin \langle m_{11}\rangle$.

(ii) In the symmetry group $4mm$ of the square, the subgroups $\langle 2, m_{10}\rangle$, $\langle 4^+\rangle$, and $\langle 2, m_{11}\rangle$ are normal subgroups because they are subgroups of index 2.
The subgroups of order 2 generated by the reflections m_{10}, m_{01}, m_{11} and $m_{1\bar{1}}$ are not normal because $4^+ \cdot m_{10} \cdot 4^- = m_{01} \notin \langle m_{10}\rangle$, $4^+ \cdot m_{01} \cdot 4^- = m_{10} \notin \langle m_{01}\rangle$, $4^+ \cdot m_{11} \cdot 4^- = m_{1\bar{1}} \notin \langle m_{11}\rangle$ and $4^+ \cdot m_{1\bar{1}} \cdot 4^- = m_{11} \notin \langle m_{1\bar{1}}\rangle$.
The subgroup of order 2 generated by the twofold rotation 2 is normal because $4^+ \cdot 2 \cdot 4^- = 2$ and $m_{10} \cdot 2 \cdot m_{10}^{-1} = 2$.

For a subgroup $\mathcal{H}$ of $\mathcal{G}$ and an element $g \in \mathcal{G}$, the conjugates ghg^{-1} form a subgroup

$$\mathcal{H}' = g\mathcal{H}g^{-1} = \{ghg^{-1} \mid h \in \mathcal{H}\}$$

because $gh_1g^{-1} \cdot gh_2g^{-1} = gh_1h_2g^{-1}$. This subgroup is called the *conjugate subgroup* of $\mathcal{H}$ by g. As already noted, conjugation does not alter the type of symmetry operations and their geometric elements, but it is possible that the orientations of the geometric elements are changed.

Using the concept of conjugate subgroups, a normal subgroup is a subgroup $\mathcal{H}$ that coincides with all its conjugate subgroups $g\mathcal{H}g^{-1}$. This means that the set of geometric elements of a normal subgroup is not changed by conjugation; the single geometric elements may, however, be permuted by the conjugating element. In the example of the symmetry group $4mm$ discussed above, the normal subgroup $\langle 2, m_{10}\rangle$ contains the reflections m_{10} and m_{01} with the lines along the coordinate axes as geometric elements. These two lines are interchanged by the fourfold rotation 4^+, corresponding to the fact that conjugation by 4^+ interchanges m_{10} and m_{01}. The concept of conjugation will be discussed in more detail in Section 1.1.8.

One of the main motivations for studying normal subgroups is that they allow us to define a group operation on the cosets of $\mathcal{H}$ in $\mathcal{G}$. The products of any element in the coset $g\mathcal{H}$ with any element in the coset $g'\mathcal{H}$ lie in a single coset, namely in the coset $gg'\mathcal{H}$. Thus we can define the product of the two cosets $g\mathcal{H}$ and $g'\mathcal{H}$ as the coset with representative gg'.

Definition. The set $\mathcal{G}/\mathcal{H} := \{g\mathcal{H} \mid g \in \mathcal{G}\}$ together with the binary operation

$$g\mathcal{H} \circ g'\mathcal{H} := gg'\mathcal{H}$$

forms a group, called the *factor group* or *quotient group* of $\mathcal{G}$ by $\mathcal{H}$.

The identity element of the factor group $\mathcal{G}/\mathcal{H}$ is the coset $\mathcal{H}$ and the inverse element of $g\mathcal{H}$ is the coset $g^{-1}\mathcal{H}$.

A familiar example of a factor group is provided by the times on a clock. If it is 8 o'clock (in the morning) now, then we say that in nine hours it will be 5 o'clock (in the afternoon). We regard times as elements of the factor group $\mathbb{Z}/12\mathbb{Z}$ in which

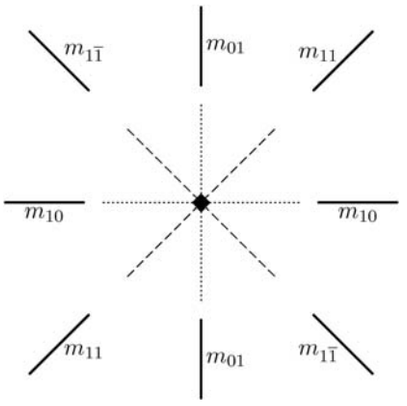

Figure 1.1.5.1
Symmetry group of an eightfold star.

$(8 + 12\mathbb{Z}) + (9 + 12\mathbb{Z}) = 17 + 12\mathbb{Z} = 5 + 12\mathbb{Z}$. In the factor group $\mathbb{Z}/12\mathbb{Z}$, the clock is imagined as a circle of circumference 12 around which the line of integers is wrapped so that integers with a difference of 12 are located at the same position on the circle.

The clock example is a special case of factor groups of the integers. We have already seen that the set $n\mathbb{Z} = \{na \mid a \in \mathbb{Z}\}$ of multiples of a natural number n forms a subgroup of index n in $\mathbb{Z}$. This is a normal subgroup, since $\mathbb{Z}$ is an abelian group. The factor group $\mathbb{Z}/n\mathbb{Z}$ represents the addition of integers *modulo n*.

Examples

(i) If we take $\mathcal{G}$ to be the symmetry group 4*mm* of the square and choose as normal subgroup the subgroup $\mathcal{H} = \langle 4^+ \rangle$ generated by the fourfold rotation, we obtain a factor group $\mathcal{G}/\mathcal{H}$ with two elements, namely the cosets $\mathcal{H} = \{1, 2, 4^+, 4^-\}$ and $m_{10}\mathcal{H} = \{m_{10}, m_{01}, m_{11}, m_{1\bar{1}}\}$. The trivial coset $\mathcal{H}$ is the identity element in the factor group $\mathcal{G}/\mathcal{H}$ and contains the rotations in 4*mm*. The other element $m_{10}\mathcal{H}$ in the factor group $\mathcal{G}/\mathcal{H}$ consists of the reflections in 4*mm*.

In this example, the separation of the rotations and reflections in 4*mm* into the two cosets $\mathcal{H}$ and $m_{10}\mathcal{H}$ makes it easy to see that the product of two cosets is independent of the chosen representative of the coset: the product of two rotations is again a rotation, hence $\mathcal{H} \cdot \mathcal{H} = \mathcal{H}$, the product of a rotation and a reflection is a reflection, hence $\mathcal{H} \cdot m_{10}\mathcal{H} = m_{10}\mathcal{H} \cdot \mathcal{H} = m_{10}\mathcal{H}$, and finally the product of two reflections is a rotation, hence $m_{10}\mathcal{H} \cdot m_{10}\mathcal{H} = \mathcal{H}$. The multiplication table of the factor group is thus

	$\mathcal{H}$	$m_{10}\mathcal{H}$
$\mathcal{H}$	$\mathcal{H}$	$m_{10}\mathcal{H}$
$m_{10}\mathcal{H}$	$m_{10}\mathcal{H}$	$\mathcal{H}$

(ii) The symmetry group of a square is the same as the symmetry group of an eightfold star, as shown in Fig. 1.1.5.1. If we regard the star as being built from four lines (two dotted and two dashed), then the twofold rotation does not move any of the lines, it only interchanges the points within each line (symmetric with respect to the centre). Regarding the lines as sets of points, the twofold rotation thus does not change anything. The effects of the different symmetry operations on the lines of the eightfold star are then precisely given by the factor group $\mathcal{G}/\mathcal{H}$, where $\mathcal{G}$ is the symmetry group 4*mm* of the square and $\mathcal{H}$ is the normal subgroup generated by the twofold rotation 2: the cosets relative to $\mathcal{H}$ are $\{1, 2\}$, $\{4^+, 4^-\}$, $\{m_{10}, m_{01}\}$, $\{m_{11}, m_{1\bar{1}}\}$, and these cosets collect together the elements of 4*mm* that have the same effect on the lines of the eightfold star. For example, both 4^+ and 4^- interchange both the two dotted and the two dashed lines, m_{10} and m_{01} both interchange the two dashed lines but fix the two dotted lines and m_{11} and $m_{1\bar{1}}$ both interchange the two dotted lines but fix the two dashed lines. Owing to the fact that $\mathcal{H}$ is a normal subgroup, the product of elements from two cosets always lies in the same coset, independent of which elements are chosen from the two cosets. For example, the product of an element from the coset $\{4^+, 4^-\}$ with an element of the coset $\{m_{10}, m_{01}\}$ always gives an element of the coset $\{m_{11}, m_{1\bar{1}}\}$. Working out the products for all pairs of cosets, one obtains the following multiplication table for the factor group $\mathcal{G}/\mathcal{H}$:

	$\{1, 2\}$	$\{4^+, 4^-\}$	$\{m_{10}, m_{01}\}$	$\{m_{11}, m_{1\bar{1}}\}$
$\{1, 2\}$	$\{1, 2\}$	$\{4^+, 4^-\}$	$\{m_{10}, m_{01}\}$	$\{m_{11}, m_{1\bar{1}}\}$
$\{4^+, 4^-\}$	$\{4^+, 4^-\}$	$\{1, 2\}$	$\{m_{11}, m_{1\bar{1}}\}$	$\{m_{10}, m_{01}\}$
$\{m_{10}, m_{01}\}$	$\{m_{10}, m_{01}\}$	$\{m_{11}, m_{1\bar{1}}\}$	$\{1, 2\}$	$\{4^+, 4^-\}$
$\{m_{11}, m_{1\bar{1}}\}$	$\{m_{11}, m_{1\bar{1}}\}$	$\{m_{10}, m_{01}\}$	$\{4^+, 4^-\}$	$\{1, 2\}$

(iii) If one takes cosets with respect to a subgroup that is not normal, the products of elements from two cosets do not lie in a single coset. As we have seen, the left cosets of the group 3*m* of an equilateral triangle with respect to the non-normal subgroup $\mathcal{H} = \{1, m_{10}\}$ are $\{1, m_{10}\}$, $\{3^+, m_{11}\}$ and $\{3^-, m_{01}\}$. Taking products from elements of the first and second coset, we get $1 \cdot 3^+ = 3^+$ and $1 \cdot m_{11} = m_{11}$, which are both in the second coset, but $m_{10} \cdot 3^+ = m_{01}$ and $m_{10} \cdot m_{11} = 3^-$, which are both in the third coset.

1.1.6. Homomorphisms, isomorphisms

In order to relate two groups, mappings between the groups that are compatible with the group operations are very useful.

Recall that a *mapping* φ from a set A to a set B associates to each $a \in A$ an element $b \in B$, denoted by $\varphi(a)$ and called the *image* of a (under φ).

Definition. For two groups $\mathcal{G}$ and $\mathcal{H}$, a mapping φ from $\mathcal{G}$ to $\mathcal{H}$ is called a *group homomorphism* or *homomorphism* for short, if it is compatible with the group operations in $\mathcal{G}$ and $\mathcal{H}$, *i.e.* if

$$\varphi(gg') = \varphi(g)\varphi(g') \text{ for all } g, g' \text{ in } \mathcal{G}.$$

The compatibility with the group operation is captured in the phrase

The image of the product is equal to the product of the images.

Fig. 1.1.6.1 gives a schematic description of the definition of a homomorphism. For φ to be a homomorphism, the two curved arrows are required to give the same result, *i.e.* first multiplying two elements in $\mathcal{G}$ and then mapping the product to $\mathcal{H}$ must be the same as first mapping the elements to $\mathcal{H}$ and then multiplying them.

It follows from the definition of a homomorphism that the identity element of $\mathcal{G}$ must be mapped to the identity element of $\mathcal{H}$ and that the inverse g^{-1} of an element $g \in \mathcal{G}$ must be mapped to the inverse of the image of g, *i.e.* that $\varphi(g^{-1}) = \varphi(g)^{-1}$. In general, however, other elements than the identity element may also be mapped to the identity element of $\mathcal{H}$.

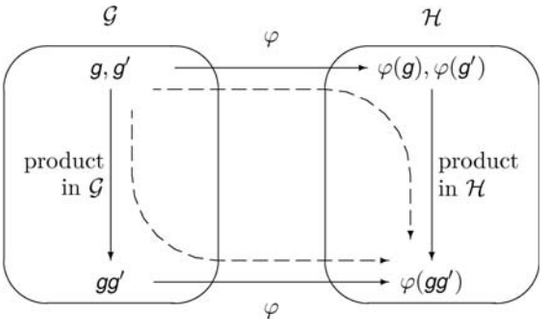

Figure 1.1.6.1
Schematic description of a homomorphism.

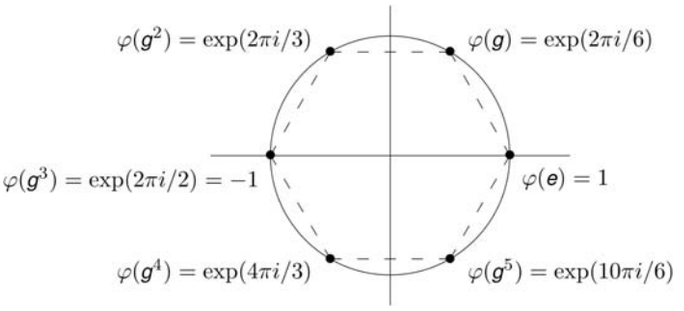

Figure 1.1.6.2
Cyclic group of order 6 embedded in the group of the unit circle.

Definition. Let φ be a group homomorphism from $\mathcal{G}$ to $\mathcal{H}$.

(i) The set $\{g \in \mathcal{G} \mid \varphi(g) = e\}$ of elements mapped to the identity element of $\mathcal{H}$ is called the *kernel* of φ, denoted by $\ker\varphi$.

(ii) The set $\varphi(\mathcal{G}) := \{\varphi(g) \mid g \in \mathcal{G}\}$ is called the *image of* $\mathcal{G}$ *under* φ.

In the case where only the identity element of $\mathcal{G}$ lies in the kernel of φ, one can conclude that $\varphi(g) = \varphi(g')$ implies $g = g'$ and φ is called an *injective homomorphism*. In this situation no information about the group $\mathcal{G}$ is lost and the homomorphism φ can be regarded as an *embedding* of $\mathcal{G}$ into $\mathcal{H}$.

The image $\varphi(\mathcal{G})$ of any homomorphism from $\mathcal{G}$ to $\mathcal{H}$ forms not just a subset, but a subgroup of $\mathcal{H}$. It is not required that $\varphi(\mathcal{G})$ is all of $\mathcal{H}$, but if this happens to be the case, φ is called a *surjective homomorphism*.

Examples

(i) For the symmetry group $4mm$ of the square a homomorphism φ to a cyclic group $\mathcal{C}_2 = \{e, g\}$ of two elements is given by $\varphi(1) = \varphi(4^+) = \varphi(2) = \varphi(4^-) = e$ and $\varphi(m_{10}) = \varphi(m_{01}) = \varphi(m_{11}) = \varphi(m_{1\bar{1}}) = g$, *i.e.* by mapping the rotations in $4mm$ to the identity element of $\mathcal{C}_2$ and the reflections to the non-trivial element.
Since every element of $\mathcal{C}_2$ is the image of some element of $4mm$, φ is a surjective homomorphism, but it is not injective because the kernel consists of all rotations in $4mm$ and not only of the identity element.

(ii) The cyclic group $\mathcal{C}_n = \{e, g, g^2, \ldots, g^{n-1}\}$ of order n is mapped into the (multiplicative) group S^1 of the unit circle in the complex plane by mapping g^k to $\exp(2\pi ik/n)$. As displayed in Fig. 1.1.6.2, the image of $\mathcal{C}_n$ under this homomorphism are points on the unit circle which form the corners of a regular n-gon.
This is an injective homomorphism because the smallest $k > 0$ with $\exp(2\pi ik/n) = 1$ is $k = n$ and $g^n = e$ in $\mathcal{C}_n$, thus by this homomorphism $\mathcal{C}_n$ can be regarded as a subgroup of S^1. It is clear that φ cannot be surjective, because S^1 is an infinite group and the image $\varphi(\mathcal{C}_n)$ consists of only finitely many elements.

(iii) For the additive group $(\mathbb{Z}, +)$ of integers and a cyclic group $\mathcal{C}_n = \{e, g, g^2, \ldots, g^{n-1}\}$, for every integer q a homomorphism φ is defined by mapping $1 \in \mathbb{Z}$ to g^q, which gives $\varphi(a) = g^{qa}$ for $a \in \mathbb{Z}$. This is never an injective homomorphism, because $n\mathbb{Z} = \{na \mid a \in \mathbb{Z}\}$ is contained in the kernel of φ. Whether or not φ is surjective depends on whether g^q is a generator of $\mathcal{C}_n$. This is the case if and only if n and q have no non-trivial common divisors.

Definition. A homomorphism φ from $\mathcal{G}$ to $\mathcal{H}$ is called an *isomorphism* if $\ker\varphi = \{e\}$ and $\varphi(\mathcal{G}) = \mathcal{H}$, *i.e.* if φ is both injective and surjective. An isomorphism is thus a one-to-one mapping between the elements of $\mathcal{G}$ and $\mathcal{H}$ which is also a homomorphism.

Groups $\mathcal{G}$ and $\mathcal{H}$ between which an isomorphism exist are called *isomorphic groups*, this is denoted by $\mathcal{G} \cong \mathcal{H}$.

Isomorphic groups may differ in the way they are realized, but they coincide in their structure. In essence, one can regard isomorphic groups as the same group with different names or labels for the group elements. For example, isomorphic groups have the same multiplication table if the elements are relabelled according to the isomorphism identifying the elements of the first group with those of the second. If one wants to stress that a certain property of a group $\mathcal{G}$ will be the same for all groups which are isomorphic to $\mathcal{G}$, one speaks of $\mathcal{G}$ as an *abstract group*.

Examples

(i) The symmetry group $3m$ of an equilateral triangle is isomorphic to the group S_3 of all permutations of $\{1, 2, 3\}$. This can be seen as follows: labelling the corners of the triangle by $1, 2, 3$, each element of $3m$ gives rise to a permutation of the labels and mapping an element to the corresponding permutation is a homomorphism. The only element fixing all three corners of the triangle is the identity element of $3m$, thus the homomorphism is injective. On the other hand, the groups $3m$ and S_3 both have 6 elements, hence the homomorphism is also surjective, and thus it is an isomorphism.

(ii) For the symmetry group $\mathcal{G} = 4mm$ of the square and its normal subgroup $\mathcal{H}$ generated by the fourfold rotation, the factor group $\mathcal{G}/\mathcal{H}$ is isomorphic to a cyclic group $\mathcal{C}_2 = \{e, g\}$ of order 2. The trivial coset (containing the rotations in $4mm$) corresponds to the identity element e, the other coset (containing the reflections) corresponds to g.

(iii) The real numbers $\mathbb{R}$ form a group with addition as operation and the positive real numbers $\mathbb{R}_{>0} = \{x \in \mathbb{R} \mid x > 0\}$ form a group with multiplication as operation. The exponential mapping $x \mapsto \exp(x)$ is a homomorphism from $(\mathbb{R}, +)$ to $(\mathbb{R}_{>0}, \cdot)$ because $\exp(x + y) = \exp(x) \cdot \exp(y)$. It is an injective homomorphisms because $\exp(x) = 1$ only for $x = 0$ [which is the identity element in $(\mathbb{R}, +)$] and it is a surjective homomorphism because for any $y > 0$ there is an $x \in \mathbb{R}$ with $\exp(x) = y$, namely $x = \log(y)$. The exponential mapping therefore provides an isomorphism from $(\mathbb{R}, +)$ to $(\mathbb{R}_{>0}, \cdot)$.

The kernel of a homomorphism φ is always a normal subgroup, since for $h \in \ker\varphi$ and $g \in \mathcal{G}$ one has $\varphi(ghg^{-1}) = \varphi(g)\varphi(h)\varphi(g^{-1}) = \varphi(g)\varphi(g^{-1}) = e$. The information about the

elements in the kernel of φ is lost after applying φ, because they are all mapped to the identity element of $\mathcal{H}$. More precisely, if $\mathcal{N} = \ker\varphi$, then all elements from the coset $g\mathcal{N}$ are mapped to the same element $\varphi(g)$ in $\mathcal{H}$, since for $n \in \mathcal{N}$ one has $\varphi(gn) = \varphi(g)\varphi(n) = \varphi(g)$. Conversely, if elements are mapped to the same element, they have to lie in the same coset, since $\varphi(g) = \varphi(g')$ implies $\varphi(g^{-1}g') = e$, thus $g^{-1}g' \in \mathcal{N}$ and thus $g^{-1}g'\mathcal{N} = \mathcal{N}$, *i.e.* $g\mathcal{N} = g'\mathcal{N}$. The cosets of $\mathcal{N}$ therefore partition the elements of $\mathcal{G}$ according to their images under φ. This observation is summarized in the following result, which is one of the most powerful theorems in group theory.

Homomorphism theorem

Let φ be a homomorphism from $\mathcal{G}$ to $\mathcal{H}$ with kernel $\ker\varphi = \mathcal{N} \trianglelefteq \mathcal{G}$. Then the factor group $\mathcal{G}/\mathcal{N}$ is isomorphic to the image $\varphi(\mathcal{G})$ *via* the isomorphism $g\mathcal{N} \mapsto \varphi(g)$.

Examples

(i) The homomorphism φ from $4mm$ to $\mathcal{C}_2 = \{e, g\}$ sending the rotations in $4mm$ to $e \in \mathcal{C}_2$ and the reflections to $g \in \mathcal{C}_2$ has the group $\mathcal{N} = \langle 4\rangle$ of rotations in $4mm$ as its kernel. The factor group $4mm/\mathcal{N}$ has the cosets $\mathcal{N} = \{1, 4^+, 2, 4^-\}$ and $m_{10}\mathcal{N} = \{m_{10}, m_{01}, m_{11}, m_{1\bar{1}}\}$ as its elements and the homomorphism theorem confirms that mapping $\mathcal{N}$ to $e \in \mathcal{C}_2$ and $m_{10}\mathcal{N}$ to $g \in \mathcal{C}_2$ is an isomorphism from $4mm/\mathcal{N}$ to $\mathcal{C}_2$.

(ii) The homomorphism φ from the additive group $(\mathbb{Z}, +)$ of integers to the cyclic group $\mathcal{C}_n = \langle g\rangle$ mapping k to g^k has $\mathcal{N} = n\mathbb{Z} = \{na \mid a \in \mathbb{Z}\}$ as its kernel. Since φ is a surjective homomorphism, the homomorphism theorem states that the factor group $\mathbb{Z}/n\mathbb{Z}$ is isomorphic to the cyclic group $\mathcal{C}_n$. The operation in the factor group $\mathbb{Z}/n\mathbb{Z}$ is 'addition *modulo n*'.

1.1.7. Group actions

The concept of a group is the essence of an abstraction process which distils the common features of various examples of groups. On the other hand, although abstract groups are important and interesting objects in their own right, they are particularly useful because the group elements *act* on something, *i.e.* they can be applied to certain objects. For example, symmetry groups act on the points in space, but they also act on lines or planes. Groups of permutations act on the symbols themselves, but also on ordered and unordered pairs. Groups of matrices act on the vectors of a vector space, but also on the subspaces. All these different actions can be described in a uniform manner and common concepts can be developed.

Definition. A *group action* of a group $\mathcal{G}$ on a set $\Omega = \{\omega \mid \omega \in \Omega\}$ assigns to each pair (g, ω) an object $\omega' = g(\omega)$ of Ω such that the following hold:

(i) applying two group elements g and g' consecutively has the same effect as applying the product $g'g$, *i.e.* $g'(g(\omega)) = (g'g)(\omega)$ (note that since the group elements act *from the left* on the objects in Ω, the elements in a product of two (or more) group elements are applied right-to-left);

(ii) applying the identity element e of $\mathcal{G}$ has no effect on ω, *i.e.* $e(\omega) = \omega$ for all ω in Ω.

One says that the object ω is *moved* to $g(\omega)$ by g.

Example

The abstract group $\mathcal{C}_2 = \{e, g\}$ occurs as symmetry group in three-dimensional space with three different actions of g:

(i) If g is a reflection, then the points fixed by g form a two-dimensional plane.

(ii) If g is a twofold rotation, then the fixed points of g form a one-dimensional line.

(iii) If g is an inversion, then only a single point is fixed by g.

Often, two objects ω and ω' are regarded as equivalent if there is a group element moving ω to ω'. This notion of equivalence is in fact an *equivalence relation* in the strict mathematical sense:

(*a*) it is *reflexive*, *i.e.* ω is equivalent to itself: this is easily seen since $e(\omega) = \omega$;

(*b*) it is *symmetric*, *i.e.* if ω is equivalent to ω', then ω' is also equivalent to ω: this holds since $g(\omega) = \omega'$ implies $g^{-1}(\omega') = \omega$;

(*c*) it is *transitive*, *i.e.* if ω is equivalent to ω' and ω' is equivalent to ω'', then ω is equivalent to ω'': this is true because $g(\omega) = \omega'$ and $g'(\omega') = \omega''$ implies $g'g(\omega) = \omega''$.

Via this equivalence relation, the action of $\mathcal{G}$ partitions the objects in Ω into equivalence classes, where the equivalence class of an object $\omega \in \Omega$ consists of all objects which are equivalent to ω.

Definition. Two objects $\omega, \omega' \in \Omega$ lie in the same *orbit* under $\mathcal{G}$ if there exists $g \in \mathcal{G}$ such that $\omega' = g(\omega)$.

The set $\mathcal{G}(\omega) := \{g(\omega) \mid g \in \mathcal{G}\}$ of all objects in the orbit of ω is called the *orbit of ω under $\mathcal{G}$*.

The set $S_{\mathcal{G}}(\omega) := \{g \in \mathcal{G} \mid g(\omega) = \omega\}$ of group elements that do not move the object ω is a subgroup of $\mathcal{G}$ called the *stabilizer* of ω in $\mathcal{G}$.

If the orbit of a group action is finite, the length of the orbit is equal to the index of the stabilizer and thus in particular a divisor of the group order (in the case of a finite group). Actually, the objects in an orbit are in a very explicit one-to-one correspondence with the cosets relative to the stabilizer, as is summarized in the *orbit–stabilizer theorem*.

Orbit–stabilizer theorem

For a group $\mathcal{G}$ acting on a set Ω let ω be an object in Ω and let $S_{\mathcal{G}}(\omega)$ be the stabilizer of ω in $\mathcal{G}$.

(i) If $g_1S_{\mathcal{G}}(\omega) \cup g_2S_{\mathcal{G}}(\omega) \cup \ldots \cup g_mS_{\mathcal{G}}(\omega)$ is the coset decomposition of $\mathcal{G}$ relative to $S_{\mathcal{G}}(\omega)$, then the coset $g_iS_{\mathcal{G}}(\omega)$ consists of precisely those elements of $\mathcal{G}$ that move ω to $g_i(\omega)$. As a consequence, the full orbit of ω is already obtained by applying only the coset representatives to ω, *i.e.* $\mathcal{G}(\omega) = \{g_1(\omega), g_2(\omega), \ldots, g_m(\omega)\}$ and the number of cosets equals the length of the orbit.

(ii) For objects in the same orbit under $\mathcal{G}$, the stabilizers are *conjugate subgroups* of $\mathcal{G}$ (*cf.* Section 1.1.5). If $\omega' = g(\omega)$, then $S_{\mathcal{G}}(\omega') = gS_{\mathcal{G}}(\omega)g^{-1}$, *i.e.* the stabilizer of ω' is obtained by conjugating the stabilizer of ω by the element g moving ω to ω'.

Example

The symmetry group $\mathcal{G} = 4mm$ of the square acts on the corners of a square as displayed in Fig. 1.1.7.1. All four points lie in a single orbit under $\mathcal{G}$ and the stabilizer of the point 1 is $\mathcal{H} = \langle m_{1\bar{1}}\rangle$, *i.e.* a subgroup of index 4, as required by the orbit–stabilizer theorem. The stabilizers of the other points are conjugate to $\mathcal{H}$: The stabilizer of corner 3 equals $\mathcal{H}$ and the stabilizer of both the corners 2 and 4 is $\langle m_{11}\rangle$, which is conjugate to $\mathcal{H}$ by the fourfold rotation 4^+ which moves corner 1 to corner 2.

An n-dimensional space group $\mathcal{G}$ acts on the points of the n-dimensional space $\mathbb{R}^n$. The stabilizer of a point $P \in \mathbb{R}^n$ is called

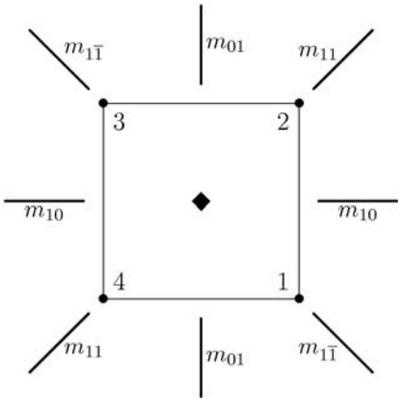

Figure 1.1.7.1
Stabilizers in the symmetry group 4*mm* of the square.

the *site-symmetry group* of P (in $\mathcal{G}$). These site-symmetry groups play a crucial role in the classification of positions in crystal structures. If the site-symmetry group of a point P consists only of the identity element of $\mathcal{G}$, P is called a point in *general position*, points with non-trivial site-symmetry groups are called points in *special position*.

According to the orbit–stabilizer theorem, points that are in the same orbit under the space group and which are thus symmetry equivalent have site-symmetry groups that are conjugate subgroups of $\mathcal{G}$. This gives rise to the concept of *Wyckoff positions*: points with site-symmetry groups that are conjugate subgroups of $\mathcal{G}$ belong to the same Wyckoff position. As a consequence, points in the same orbit under $\mathcal{G}$ certainly belong to the same Wyckoff position, but points may have the same site-symmetry group without being symmetry equivalent. The Wyckoff position of a point P consists of the union of the orbits of all points Q that have the same site-symmetry group as P. For a detailed discussion of the crucial notion of Wyckoff positions we refer to Section 1.4.4.

Example

In the symmetry group 4*mm* of the square the points $x, 0$ lying on the geometric element of m_{01} (*i.e.* the reflection line) are clearly stabilized by m_{01}. The origin $0, 0$ has the full group 4*mm* as its site-symmetry group, for all other points $x, 0$ with $x \neq 0$ the site-symmetry group is the group $\langle m_{01} \rangle$ generated by the reflection m_{01}.

The orbit of a point $P = x, 0$ with $x \neq 0$ is the four points $x, 0$, $0, x$, $-x, 0$, $0, -x$, where both $x, 0$ and $-x, 0$ have site-symmetry group $\langle m_{01} \rangle$ and $0, x$ and $0, -x$ have the conjugate site-symmetry group $\langle m_{10} \rangle$. This means that the Wyckoff position of *e.g.* the point $P = \frac{1}{2}, 0$ consists of the set of all points $x, 0$ and $0, x$ with arbitrary $x \neq 0$, *i.e.* of the union of the geometric elements of m_{01} and m_{10} with the exception of their intersection $0, 0$. A complete description of the distribution of points among the Wyckoff positions of the group 4*mm* is given in Table 3.2.3.1.

1.1.8. Conjugation, normalizers

In this section we focus on two group actions which are of particular importance for describing intrinsic properties of a group, namely the conjugation of group elements and the conjugation of subgroups. These actions were mentioned earlier in Section 1.1.5 when we introduced normal subgroups.

A group $\mathcal{G}$ acts on its elements *via* $g(h) := ghg^{-1}$, *i.e.* by conjugation. Note that the inverse element g^{-1} is required on the right-hand side of h in order to fulfil the rule $g(g'(h)) = (gg')(h)$ for a group action.

The orbits for this action are called the *conjugacy classes of elements* of $\mathcal{G}$ or simply *conjugacy classes* of $\mathcal{G}$; the conjugacy class of an element h consists of all its conjugates ghg^{-1} with g running over all elements of $\mathcal{G}$. Elements in one conjugacy class have *e.g.* the same order, and in the case of groups of symmetry operations they also share geometric properties such as being a reflection, rotation or rotoinversion. In particular, conjugate elements have the same type of geometric element.

The connection between conjugate symmetry operations and their geometric elements is even more explicit by the orbit–stabilizer theorem: If h and h' are conjugate by g, *i.e.* $h' = ghg^{-1}$, then g maps the geometric element of h to the geometric element of h'.

Example

The rotation group of a cube contains six fourfold rotations and if the cube is in standard orientation with the origin in its centre, the fourfold rotations 4^+_{100}, 4^+_{010} and 4^+_{001} and their inverses have the lines along the coordinate axes

$$\left\{ \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix} \mid x \in \mathbb{R} \right\}, \left\{ \begin{pmatrix} 0 \\ y \\ 0 \end{pmatrix} \mid y \in \mathbb{R} \right\} \text{ and } \left\{ \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix} \mid z \in \mathbb{R} \right\}$$

as their geometric elements, respectively. The twofold rotation 2_{110} around the line

$$\left\{ \begin{pmatrix} x \\ x \\ 0 \end{pmatrix} \mid x \in \mathbb{R} \right\}$$

maps the a axis to the b axis and *vice versa*, therefore the symmetry operation 2_{110} conjugates 4^+_{100} to a fourfold rotation with the line along the b axis as geometric element. Since the positive part of the a axis is mapped to the positive part of the b axis and conjugation also preserves the handedness of a rotation, 4^+_{100} is conjugated to 4^+_{010} and not to the inverse element 4^-_{010}. The line along the c axis is fixed by 2_{110}, but its orientation is reversed, *i.e.* the positive and negative parts of the c axis are interchanged. Therefore, 4^+_{001} is conjugated to its inverse 4^-_{001} by 2_{110}.

For the conjugation action, the stabilizer of an element h is called the *centralizer* $\mathcal{C}_{\mathcal{G}}(h)$ of h in $\mathcal{G}$, consisting of all elements in $\mathcal{G}$ that commute with h, *i.e.* $\mathcal{C}_{\mathcal{G}}(h) = \{g \in \mathcal{G} \mid gh = hg\}$.

Elements that form a conjugacy class on their own commute with all elements of $\mathcal{G}$ and thus have the full group as their centralizer. The collection of all these elements forms a normal subgroup of $\mathcal{G}$ which is called the *centre* of $\mathcal{G}$.

A group $\mathcal{G}$ acts on its subgroups *via* $g(\mathcal{H}) := g\mathcal{H}g^{-1} = \{ghg^{-1} \mid h \in \mathcal{H}\}$, *i.e.* by conjugating all elements of the subgroup. The orbits are called *conjugacy classes of subgroups* of $\mathcal{G}$. Considering the conjugation action of $\mathcal{G}$ on its subgroups is often convenient, because conjugate subgroups are in particular isomorphic: an isomorphism from $\mathcal{H}$ to $g\mathcal{H}g^{-1}$ is provided by the mapping $h \mapsto ghg^{-1}$.

The stabilizer of a subgroup $\mathcal{H}$ of $\mathcal{G}$ under this conjugation action is called the *normalizer* $\mathcal{N}_{\mathcal{G}}(\mathcal{H})$ of $\mathcal{H}$ in $\mathcal{G}$. The normalizer of a subgroup $\mathcal{H}$ of $\mathcal{G}$ is the largest subgroup $\mathcal{N}$ of $\mathcal{G}$ such that $\mathcal{H}$ is a normal subgroup of $\mathcal{N}$. In particular, a subgroup is a normal subgroup of $\mathcal{G}$ if and only if its normalizer is the full group $\mathcal{G}$.

The number of conjugate subgroups of $\mathcal{H}$ in $\mathcal{G}$ is equal to the index of $\mathcal{N}_\mathcal{G}(\mathcal{H})$ in $\mathcal{G}$. According to the orbit–stabilizer theorem, the different conjugate subgroups of $\mathcal{H}$ are obtained by conjugating $\mathcal{H}$ with coset representatives for the cosets of $\mathcal{G}$ relative to $\mathcal{N}_\mathcal{G}(\mathcal{H})$.

Examples

(i) In an abelian group $\mathcal{G}$, every element is only conjugate with itself, since $ghg^{-1} = h$ for all g, h in $\mathcal{G}$. Therefore each conjugacy class consists of just a single element.
Also, every subgroup $\mathcal{H}$ of an abelian group $\mathcal{G}$ is a normal subgroup, thus its normalizer $\mathcal{N}_\mathcal{G}(\mathcal{H})$ is $\mathcal{G}$ itself and $\mathcal{H}$ is only conjugate to itself.

(ii) The conjugacy classes of the symmetry group $3m$ of an equilateral triangle are $\{1\}$, $\{m_{10}, m_{01}, m_{11}\}$ and $\{3^+, 3^-\}$. The centralizer of m_{10} is just the group $\langle m_{10}\rangle$ generated by m_{10}, *i.e.* 1 and m_{10} are the only elements of $3m$ commuting with m_{10}. Analogously, one sees that the centralizer $\mathcal{C}_\mathcal{G}(h) = \langle h\rangle$ for each element h in $3m$, except for $h = 1$.
The subgroups $\langle m_{10}\rangle$, $\langle m_{01}\rangle$ and $\langle m_{11}\rangle$ are conjugate subgroups (with conjugating elements 3^+ and 3^-). These subgroups coincide with their normalizers, since they have index 3 in the full group.

(iii) The conjugacy classes of the symmetry group $4mm$ of a square are $\{1\}$, $\{2\}$, $\{m_{10}, m_{01}\}$, $\{m_{11}, m_{1\bar{1}}\}$ and $\{4^+, 4^-\}$. Since 2 forms a conjugacy class on its own, this is an element in the centre of $4mm$ and its centralizer is the full group. The centralizer of m_{10} is $\langle m_{10}, m_{01}\rangle$, which is also the centralizer of m_{01} (note that m_{10} and m_{01} are reflections with normal vectors perpendicular to each other, and thus commute). Analogously, $\langle m_{11}, m_{1\bar{1}}\rangle$ is the centralizer of both m_{11} and $m_{1\bar{1}}$. Finally, 4^+ only commutes with the rotations in $4mm$, therefore its centralizer is $\langle 4^+\rangle$.
The five subgroups of order 2 in $4mm$ fall into three conjugacy classes, namely the normal subgroup $\langle 2\rangle$ and the two pairs $\{\langle m_{10}\rangle, \langle m_{01}\rangle\}$ and $\{\langle m_{11}\rangle, \langle m_{1\bar{1}}\rangle\}$. The normalizer of both $\langle m_{10}\rangle$ and $\langle m_{01}\rangle$ is $\langle 2, m_{10}\rangle$ and the normalizer of both $\langle m_{11}\rangle$ and $\langle m_{1\bar{1}}\rangle$ is $\langle 2, m_{11}\rangle$.

In the context of crystallographic groups, conjugate subgroups are not only isomorphic, but have the same types of geometric elements, possibly with different directions. In many situations it is therefore sufficient to restrict attention to representatives of the conjugacy classes of subgroups. Furthermore, conjugation with elements from the normalizer of a group $\mathcal{H}$ permutes the geometric elements of the symmetry operations of $\mathcal{H}$. The role of the normalizer may in this situation be expressed by the phrase

The normalizer describes the *symmetry of the symmetries*.

Thus, the normalizer reflects an intrinsic ambiguity between different but equivalent descriptions of an object by its symmetries.

Example

The subgroup $\mathcal{H} = \langle 2, m_{10}\rangle$ is a normal subgroup of the symmetry group $\mathcal{G} = 4mm$ of the square, and thus $\mathcal{G}$ is the normalizer of $\mathcal{H}$ in $\mathcal{G}$. As can be seen in the diagram in Fig. 1.1.7.1, the fourfold rotation 4^+ maps the geometric element of the reflection m_{10} to the geometric element of m_{01} and *vice versa*, and fixes the geometric element of the rotation 4^+. Consequently, conjugation by 4^+ fixes $\mathcal{H}$ as a set, but interchanges the reflections m_{10} and m_{01}. These two reflections are geometrically indistinguishable, since their geometric elements are both lines through the centres of opposite edges of the square.
Analogously, 4^+ interchanges the geometric elements of the reflections m_{11} and $m_{1\bar{1}}$ of the subgroup $\mathcal{H}' = \langle 2, m_{11}\rangle$. These are the two reflection lines through opposite corners of the square.
In contrast to that, $\mathcal{G}$ does not contain an element mapping the geometric element of m_{10} to that of m_{11}. Note that an eightfold rotation would be such an element, but this is, however, not a symmetry of the square. The reflections m_{10} and m_{11} are thus geometrically different symmetry operations of the square.

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1.2. Crystallographic symmetry

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1.2.1. Crystallographic symmetry operations

Geometric mappings have the property that for each point P of the space, and thus of the object, there is a uniquely determined point $\tilde{P}$, the *image point*. If also for each image point $\tilde{P}$ there is a uniquely determined preimage or original point P, then the mapping is called *reversible*. Non-reversible mappings are called *projections*, *cf.* Section 1.4.5.

A mapping is called a *motion*, a *rigid motion* or an *isometry* if it leaves all distances invariant (and thus all angles, as well as the size and shape of an object). In this volume the term 'isometry' is used.

Isometries are a special kind of affine mappings. In an *affine mapping*, parallel lines are mapped onto parallel lines; lengths and angles may be distorted but distances along the same line are preserved.

A mapping is called a *symmetry operation* of an object if (i) it is an isometry, and (ii) it maps the object onto itself. Instead of 'maps the object onto itself' one frequently says 'leaves the object invariant (as a whole)'.

Real crystals are finite objects in physical space, which because of the presence of impurities and structural imperfections such as disorder, dislocations *etc*. are not perfectly symmetric. In order to describe their symmetry properties, real crystals are modelled as blocks of ideal, infinitely extended periodic structures, known as *ideal crystals* or (ideal) crystal structures. Crystal patterns are models of crystal structures in point space. In other words, while the crystal structure is an infinite periodic spatial arrangement of the atoms (ions, molecules) of which the real crystal is composed, the crystal pattern is the related model of the ideal crystal (crystal structure) consisting of a strictly three-dimensional periodic set of points in point space. If the growth of the ideal crystal is undisturbed, then it forms an *ideal macroscopic crystal* and displays its ideal shape with planar faces.

Both the symmetry operations of an ideal crystal and of a crystal pattern are called *crystallographic symmetry operations*. The symmetry operations of the ideal macroscopic crystal form the finite point group of the crystal, those of the crystal pattern form the (infinite) space group of the crystal pattern. Because of its periodicity, a crystal pattern always has translations among its symmetry operations.

The symmetry operations are divided into two main kinds depending whether they preserve or not the so-called *handedness* or *chirality* of chiral objects. *Isometries of the first kind* or *proper isometries* are those that preserve the handedness of chiral objects: *e.g.* if a right (left) glove is mapped by one of these isometries, then the image is also a right (left) glove of equal size and shape. Isometries that change the handedness, *i.e.* the image of a right glove is a left one, of a left glove is a right one, are called *isometries of the second kind* or *improper isometries*. Improper isometries cannot be performed in space physically but can nevertheless be observed as symmetries of objects.

The notion of *fixed points* is essential for the characterization of symmetry operations. A point P is a *fixed point* of a mapping if it is mapped onto itself, *i.e.* the *image point* $\tilde{P}$ is the same as the original point P: $\tilde{P} = P$. The set of all fixed points of an isometry may be the whole space, a plane in the space, a straight line, a point, or the set may be empty (no fixed point).

Crystallographic symmetry operations are also characterized by their *order*: a symmetry operation W is of *order* k if its application k times results in the identity mapping, *i.e* $\mathsf{W}^k = \mathsf{I}$, where I is the identity operation, and $k > 0$ is the smallest number for which this equation is fulfilled.

There are eight different types of isometries that may be crystallographic symmetry operations:

(1) The *identity operation* I maps each point of the space onto itself, *i.e.* the set of fixed points is the whole space. It is the only operation whose order is 1. The identity operation is a symmetry operation of the first kind. It is a symmetry operation of any object and although trivial, it is indispensable for the group properties of the set of symmetry operations of the object (*cf.* Section 1.1.2).

(2) A *translation* t is characterized by its translation vector $\mathbf{t}$. Under translation every point of space is shifted by $\mathbf{t}$, hence a translation has no fixed point. A translation is a symmetry operation of infinite order as there is no number $k \neq 0$ such that $t^k = \mathsf{I}$ with translation vector $\mathbf{o}$. It preserves the handedness of any chiral object.

(3) A *rotation* is an isometry which leaves one line fixed pointwise. This line is called the *rotation axis*. The degree of rotation about this axis is described by its rotation angle ϕ. Because of the periodicity of crystals, the rotation angles of crystallographic rotations are restricted to $\phi = k \times 2\pi/N$, where N = 2, 3, 4 or 6 and k is an integer which is relative prime to N. A rotation of rotation angle $\phi = k \times 2\pi/N$ is of order N and is called an N-fold rotation. A rotation preserves the handedness of any chiral object.

The rotations are also characterized by their *sense of rotation*. The adopted convention for *positive* (*negative*) sense of rotation follows the mathematical convention for *positive* (*negative*) sense of rotation: the sense of rotation is positive (negative) if the rotation is counter-clockwise (clockwise) when viewed down the rotation axis.

(4) A *screw rotation* is a rotation coupled with a translation parallel to the rotation axis. The rotation axis is called the *screw axis*. The translation vector is called the *screw vector* or the *intrinsic translation component* $\boldsymbol{w}_g$ (of the screw rotation), *cf.* Section 1.2.2.4. A screw rotation has no fixed points because of its translation component. However, the screw axis is invariant pointwise under the so-called *reduced symmetry operation* of the screw rotation: it is the rotation obtained from the screw rotation by removing its intrinsic translation component.

The screw rotation is a proper symmetry operation. If $\phi = 2\pi/N$ is the smallest rotation angle of a screw rotation, then the screw rotation is called N-fold. Owing to its translation component, the order of any screw rotation is infinite. Let $\mathbf{u}$ be the shortest lattice vector in the direction of the screw axis, and $n\mathbf{u}/N$, with $n \neq 0$ and integer, be the screw

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vector of the screw rotation by the angle ϕ. After N screw rotations with rotation angle $\phi = 2\pi/N$ the crystal pattern has its original orientation but is shifted parallel to the screw axis by the lattice vector $n\mathbf{u}$.

(5) An N-fold *rotoinversion* $\overline{N}$ is an N-fold rotation coupled with an inversion through a point on the rotation axis. This point is called the *centre of the rotoinversion*. For $N \neq 2$ it is the only fixed point. The axis of the rotation is invariant as a whole under the rotoinversion and is called its *rotoinversion axis*. The restrictions on the angles ϕ of the rotational parts are the same as for rotations. The order of an *N-fold* rotoinversion is N for even N and $2N$ for odd N. A rotoinversion changes the handedness by its inversion component: it maps any right-hand glove onto a left-hand one and *vice versa*. Special rotoinversions are those for $N = 1$ and $N = 2$ which are dealt with separately.

The rotoinversions $\overline{N}$ can be described equally as roto-reflections S_N. The N-fold rotation is now coupled with a reflection through a plane which is perpendicular to the rotation axis and cuts the axis in its centre. The following equivalences hold: $\bar{1} = S_2$, $\bar{2} = m = S_1$, $\bar{3} = S_6^{-1}$, $\bar{4} = S_4^{-1}$ and $\bar{6} = S_3^{-1}$. In this volume the description by rotoinversions is chosen.

(6) The *inversion* can be considered as a onefold rotoinversion ($\bar{1}$, $N = 1$) or equally as a twofold rotoreflection S_2. The fixed point is called the *inversion centre*. The inversion is a symmetry operation of the second kind, its order is 2.

(7) A twofold rotoinversion ($N = 2$) is equivalent to a *reflection* or a *reflection through a plane* and is simultaneously a onefold rotoreflection ($\bar{2} = m = S_1$). It is an isometry which leaves the plane perpendicular to the twofold rotoinversion axis fixed pointwise. This plane is called the *reflection plane* or *mirror plane*; it intersects the rotation axis in its centre. Its orientation is described by the direction of its normal vector, *i.e.* of the rotation axis. (Note that in the space-group tables of Part 2 the reflection planes are specified by their locations, and not by their normal vectors, *cf.* Section 1.4.2.1.) The order of a reflection is 2. As for any rotoinversion, the reflection changes the handedness of a chiral object.

(8) A *glide reflection* is a reflection through a plane coupled with a translation parallel to this plane. The translation vector is called the *glide vector* (or the *intrinsic translation component* $\boldsymbol{w}_g$ of the glide reflection, *cf.* Section 1.2.2.4). A glide reflection changes the handedness and has no fixed point. The set of fixed points of the related reduced symmetry operation (*i.e.* the reflection that is obtained by removing the glide component from the glide reflection) is called the *glide plane*. The glide vector of a glide reflection is 1/2 of a lattice vector $\mathbf{t}$ (including centring translations of centred-cell lattice descriptions, *cf.* Table 2.1.1.2). Whereas twice the application of a reflection restores the original position of the crystal pattern, applying a glide reflection twice results in a translation of the crystal pattern with the translation vector $\mathbf{t} = 2\boldsymbol{w}_g$. The order of any glide reflection is infinite.

1.2.2. Matrix description of symmetry operations[1]

1.2.2.1. Matrix–column presentation of isometries

In order to describe mappings analytically one introduces a coordinate system $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$, consisting of three linearly independent (*i.e.* not coplanar) basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ (or $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$) and an origin O. Referred to this coordinate system each point P can be described by three coordinates x, y, z (or x_1, x_2, x_3). A mapping can be regarded as an instruction for how to calculate the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$ of the image point $\widetilde{X}$ from the coordinates x, y, z of the original point X.

The instruction for the calculation of the coordinates of $\widetilde{X}$ from the coordinates of X is simple for an affine mapping and thus for an isometry. The equations are

$$\begin{aligned} \tilde{x} &= W_{11}x + W_{12}y + W_{13}z + w_1 \\ \tilde{y} &= W_{21}x + W_{22}y + W_{23}z + w_2 \\ \tilde{z} &= W_{31}x + W_{32}y + W_{33}z + w_3, \end{aligned} \qquad (1.2.2.1)$$

where the coefficients W_{ik} and w_j are constant. These equations can be written using the matrix formalism:

$$\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}. \qquad (1.2.2.2)$$

This matrix equation is usually abbreviated by

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}, \qquad (1.2.2.3)$$

where

$$\tilde{\boldsymbol{x}} = \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix}, \ \boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \ \boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \text{ and}$$

$$\boldsymbol{W} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix}.$$

The matrix $\boldsymbol{W}$ is called the *linear part* or *matrix part* and the column $\boldsymbol{w}$ is the *translation part* or *column part* of the mapping. The rotation parts $\boldsymbol{W}$ referring to conventional coordinate systems of all space-group symmetry operations are listed in Tables 1.2.2.1 and 1.2.2.2 as matrices for point-group symmetry operations.

Very often, equation (1.2.2.3) is written in the form

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} \ \text{ or } \ \tilde{\boldsymbol{x}} = \{\boldsymbol{W} \mid \boldsymbol{w}\}\boldsymbol{x}. \qquad (1.2.2.4)$$

The symbols $(\boldsymbol{W}, \boldsymbol{w})$ and $\{\boldsymbol{W} \mid \boldsymbol{w}\}$ which describe the mapping referred to the chosen coordinate system are called the *matrix–column pair* and can be considered as *Seitz symbols* (Seitz, 1935) (*cf.* Section 1.4.2.2 for an introduction to and listings of Seitz symbols of crystallographic symmetry operations).

1.2.2.1.1. Shorthand notation of matrix–column pairs

In crystallography in general, and in this volume in particular, an efficient procedure is used to condense the description of symmetry operations by matrix–column pairs considerably. The so-called *shorthand notation* of the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ consists of a coordinate triplet $W_{11}x + W_{12}y + W_{13}z + w_1$, $W_{21}x + W_{22}y + W_{23}z + w_2$, $W_{31}x + W_{32}y + W_{33}z + w_3$. All coefficients '+1' and the terms with coefficients 0 are omitted, while coefficients '−1' are replaced by '−' and are frequently written on top of the variable: $\overline{x}$ instead of $-x$ *etc.* The following examples illustrate the assignments of the coordinate triplets to the matrix–column pairs.

Examples

(1) The coordinate triplet of $y + 1/2, \overline{x} + 1/2, z + 1/4$ stands for the symmetry operation with the rotation part

[1] With Tables 1.2.2.1 and 1.2.2.2 by H. Arnold.

Table 1.2.2.1
Matrices for point-group symmetry operations and orientation of corresponding geometric elements, referred to a cubic, tetragonal, orthorhombic, monoclinic, triclinic or rhombohedral coordinate system

Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 $0, 0, z$ [001]	$\bar{x}, \bar{y}, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	2 $0, y, 0$ [010]	$\bar{x}, y, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 0, 0$ [100]	$x, \bar{y}, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
3^+ x, x, x [111]	z, x, y	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	3^+ $x, \bar{x}, \bar{x}$ [1$\bar{1}\bar{1}$]	$\bar{z}, \bar{x}, y$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	3^+ $\bar{x}, x, \bar{x}$ [$\bar{1}$1$\bar{1}$]	$z, \bar{x}, \bar{y}$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$	3^+ $\bar{x}, \bar{x}, x$ [$\bar{1}\bar{1}$1]	$\bar{z}, x, \bar{y}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$
3^- x, x, x [111]	y, z, x	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	3^- $x, \bar{x}, \bar{x}$ [1$\bar{1}\bar{1}$]	$\bar{y}, z, \bar{x}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}$	3^- $\bar{x}, x, \bar{x}$ [$\bar{1}$1$\bar{1}$]	$\bar{y}, \bar{z}, x$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	3^- $\bar{x}, \bar{x}, x$ [$\bar{1}\bar{1}$1]	$y, \bar{z}, \bar{x}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}$
			2 $x, x, 0$ [110]	$y, x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 0, x$ [101]	$z, \bar{y}, x$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$	2 $0, y, y$ [011]	$\bar{x}, z, y$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
			2 $x, \bar{x}, 0$ [1$\bar{1}$0]	$\bar{y}, \bar{x}, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $\bar{x}, 0, x$ [$\bar{1}$01]	$\bar{z}, \bar{y}, \bar{x}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	2 $0, y, \bar{y}$ [01$\bar{1}$]	$\bar{x}, \bar{z}, \bar{y}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \end{pmatrix}$
			4^+ $0, 0, z$ [001]	$\bar{y}, x, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	4^+ $0, y, 0$ [010]	$z, y, \bar{x}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	4^+ $x, 0, 0$ [100]	$x, \bar{z}, y$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$
			4^- $0, 0, z$ [001]	$y, \bar{x}, z$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	4^- $0, y, 0$ [010]	$\bar{z}, y, x$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	4^- $x, 0, 0$ [100]	$x, z, \bar{y}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$
$\bar{1}$ $0, 0, 0$	$\bar{x}, \bar{y}, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	m $x, y, 0$ [001]	$x, y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	m $x, 0, z$ [010]	$x, \bar{y}, z$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $0, y, z$ [100]	$\bar{x}, y, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$\bar{3}^+$ x, x, x [111]	$\bar{z}, \bar{x}, \bar{y}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$	$\bar{3}^+$ $x, \bar{x}, \bar{x}$ [1$\bar{1}\bar{1}$]	$z, x, \bar{y}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$	$\bar{3}^+$ $\bar{x}, x, \bar{x}$ [$\bar{1}$1$\bar{1}$]	$\bar{z}, x, y$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\bar{3}^+$ $\bar{x}, \bar{x}, x$ [$\bar{1}\bar{1}$1]	$z, \bar{x}, y$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
$\bar{3}^-$ x, x, x [111]	$\bar{y}, \bar{z}, \bar{x}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\bar{3}^-$ $x, \bar{x}, \bar{x}$ [1$\bar{1}\bar{1}$]	$y, \bar{z}, x$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	$\bar{3}^-$ $\bar{x}, x, \bar{x}$ [$\bar{1}$1$\bar{1}$]	$y, z, \bar{x}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\bar{3}^-$ $\bar{x}, \bar{x}, x$ [$\bar{1}\bar{1}$1]	$\bar{y}, z, x$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
			m $x, \bar{x}, z$ [110]	$\bar{y}, \bar{x}, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $\bar{x}, y, x$ [101]	$\bar{z}, y, \bar{x}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	m $x, y, \bar{y}$ [011]	$x, \bar{z}, \bar{y}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \end{pmatrix}$
			m x, x, z [1$\bar{1}$0]	y, x, z	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m x, y, x [$\bar{1}$01]	z, y, x	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	m x, y, y [01$\bar{1}$]	x, z, y	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
			$\bar{4}^+$ $0, 0, z$ [001]	$y, \bar{x}, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{4}^+$ $0, y, 0$ [010]	$\bar{z}, \bar{y}, x$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\bar{4}^+$ $x, 0, 0$ [100]	$\bar{x}, z, \bar{y}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$
			$\bar{4}^-$ $0, 0, z$ [001]	$\bar{y}, x, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{4}^-$ $0, y, 0$ [010]	$z, \bar{y}, \bar{x}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\bar{4}^-$ $x, 0, 0$ [100]	$\bar{x}, \bar{z}, y$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$

Table 1.2.2.2
Matrices for point-group symmetry operations and orientation of corresponding geometric elements, referred to a hexagonal coordinate system

Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$	Symbol of symmetry operation and orientation of geometric element	Transformed coordinates $\tilde{x}, \tilde{y}, \tilde{z}$	Matrix $\boldsymbol{W}$
1	x, y, z	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3^+ 0, 0, z [001]	$\bar{y}, x-y, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	3^- 0, 0, z [001]	$y-x, \bar{x}, z$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
2 0, 0, z [001]	$\bar{x}, \bar{y}, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	6^+ 0, 0, z [001]	$x-y, x, z$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	6^- 0, 0, z [001]	$y, y-x, z$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
2 $x, x, 0$ [110]	$y, x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 0, 0$ [100]	$x-y, \bar{y}, \bar{z}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $0, y, 0$ [010]	$\bar{x}, y-x, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
2 $x, \bar{x}, 0$ [1$\bar{1}$0]	$\bar{y}, \bar{x}, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $x, 2x, 0$ [120]	$y-x, y, \bar{z}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	2 $2x, x, 0$ [210]	$x, x-y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
$\bar{1}$ 0, 0, 0	$\bar{x}, \bar{y}, \bar{z}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{3}^+$ 0, 0, z [001]	$y, y-x, \bar{z}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{3}^-$ 0, 0, z [001]	$x-y, x, \bar{z}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
m $x, y, 0$ [001]	$x, y, \bar{z}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{6}^+$ 0, 0, z [001]	$y-x, \bar{x}, \bar{z}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\bar{6}^-$ 0, 0, z [001]	$\bar{y}, x-y, \bar{z}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$
m $x, \bar{x}, z$ [110]	$\bar{y}, \bar{x}, z$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $x, 2x, z$ [100]	$y-x, y, z$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $2x, x, z$ [010]	$x, x-y, z$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$
m x, x, z [1$\bar{1}$0]	y, x, z	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $x, 0, z$ [120]	$x-y, \bar{y}, z$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	m $0, y, z$ [210]	$\bar{x}, y-x, z$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$$\boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the translation part $\boldsymbol{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/4 \end{pmatrix}$. The assignment of the coordinate triplet to the matrix–column pair becomes obvious if one applies the equations (1.2.2.2) for the specific case of $(\boldsymbol{W}, \boldsymbol{w})$:

$$\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ 1/4 \end{pmatrix}$$

would be

$$\tilde{x} = 0x + 1y + 0z + 1/2, \quad \tilde{y} = -1x + 0y + 0z + 1/2,$$
$$\tilde{z} = 0x + 0y + 1z + 1/4.$$

This symmetry operation is found under space group $P4_32_12$, No. 96 in the space-group tables of Chapter 2.3. It is the entry (4) of the first block (the so-called *General position* block) starting with 8 *b* 1 under the heading **Positions**.

(2) The matrix–column pair

$$(\boldsymbol{W}, \boldsymbol{w}) = \left(\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix} \right)$$

is represented in shorthand notation by the coordinate triplet $\bar{x} + y, y, \bar{z} + 1/2$. This is the entry (11) of the general positions of the space group $P6_522$, No. 179 (*cf.* the space-group tables of Chapter 2.3).

1.2.2.2. Combination of mappings and inverse mappings

The combination of two symmetry operations $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ is again a symmetry operation. The linear and translation part of the combined symmetry operation is derived from the rotation and translation parts of $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ in a straightforward way:

Applying first the symmetry operation $(\boldsymbol{W}_1, \boldsymbol{w}_1)$, on the one hand,

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1,$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{W}_2\tilde{\boldsymbol{x}} + \boldsymbol{w}_2 = \boldsymbol{W}_2(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1) + \boldsymbol{w}_2 = \boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2. \quad (1.2.2.5)$$

On the other hand

$$\tilde{\tilde{\boldsymbol{x}}} = (\boldsymbol{W}_2, \boldsymbol{w}_2)\tilde{\boldsymbol{x}} = (\boldsymbol{W}_2, \boldsymbol{w}_2)(\boldsymbol{W}_1, \boldsymbol{w}_1)\boldsymbol{x}. \quad (1.2.2.6)$$

By comparing equations (1.2.2.5) and (1.2.2.6) one obtains

$$(\boldsymbol{W}_2, \boldsymbol{w}_2)(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1, \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2). \quad (1.2.2.7)$$

The formula for the inverse of an affine mapping follows from the equations $\tilde{\boldsymbol{x}} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}$, *i.e.* $\boldsymbol{x} = \boldsymbol{W}^{-1}\tilde{\boldsymbol{x}} - \boldsymbol{W}^{-1}\boldsymbol{w}$, which compared with $\boldsymbol{x} = (\boldsymbol{W}, \boldsymbol{w})^{-1}\tilde{\boldsymbol{x}}$ gives

$$(\boldsymbol{W}, \boldsymbol{w})^{-1} = (\boldsymbol{W}^{-1}, -\boldsymbol{W}^{-1}\boldsymbol{w}). \quad (1.2.2.8)$$

Because of the inconvenience of these relations, especially for the column parts of the isometries, it is often preferable to use so-called *augmented matrices*, by which one can describe the combination of affine mappings and the inverse mapping by equations of matrix multiplication. These matrices are introduced in the following section.

1.2.2.3. Matrix–column pairs and (3 + 1) × (3 + 1) matrices

It is natural to combine the matrix part and the column part describing an affine mapping to form a (3 × 4) matrix, but such matrices cannot be multiplied by the usual matrix multiplication and cannot be inverted. However, if one supplements the (3 × 4) matrix by a fourth row '0 0 0 1', one obtains a (4 × 4) square matrix which can be combined with the analogous matrices of other mappings and can be inverted. These matrices are called *augmented matrices*, and here they are designated by open-face letters. Similarly, the columns $\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}$ also have to be extended to the augmented columns $\mathbb{x}$ and $\tilde{\mathbb{x}}$:

$$\mathbb{W} = \left(\begin{array}{cccc} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \quad \tilde{\mathbb{x}} = \left(\begin{array}{c} \tilde{x} \\ \tilde{y} \\ \tilde{z} \\ \hline 1 \end{array}\right), \quad \mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right). \tag{1.2.2.9}$$

The horizontal and vertical lines in the augmented matrices are useful to facilitate recognition of their coefficients; they have no mathematical meaning.

Equations (1.2.2.1), (1.2.2.7) and (1.2.2.8) then become

$$\tilde{\mathbb{x}} = \mathbb{W}\mathbb{x}, \tag{1.2.2.10}$$

$$\mathbb{W}_3 = \mathbb{W}_2\mathbb{W}_1 \quad \text{and} \quad (\mathbb{W})^{-1} = (\mathbb{W}^{-1}). \tag{1.2.2.11}$$

In the usual description by columns, the vector coefficients cannot be distinguished from the point coordinates, but in the augmented-column description the difference becomes visible.

If $\mathbb{p}$ and $\mathbb{q}$ are the augmented columns of coordinates of the points P and Q, $\mathbb{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ \hline 1 \end{pmatrix}$ and $\mathbb{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ \hline 1 \end{pmatrix}$, then $\mathbb{v} = \begin{pmatrix} q_1 - p_1 \\ q_2 - p_2 \\ q_3 - p_3 \\ \hline 0 \end{pmatrix}$ is the augmented column $\mathbb{v}$ of the coefficients of the vector $\mathbf{v}$ between P and Q. The last coefficient of $\mathbb{v}$ is zero, because $1 - 1 = 0$. Thus, the column of the coefficients of a vector is not augmented by '1' but by '0'. From the equation for the transformation of the vector coefficients $\tilde{\mathbb{v}} = \mathbb{W}\mathbb{v}$ it becomes clear that when the point P is mapped onto the point $\tilde{P}$ by $\tilde{\boldsymbol{x}} = \boldsymbol{W}\underrightarrow{\boldsymbol{x}} + \boldsymbol{w}$ according to equation (1.2.2.3), then the vector $\mathbf{v} = \underrightarrow{PQ}$ is mapped onto the vector $\tilde{\mathbf{v}} = \underrightarrow{\tilde{P}\tilde{Q}}$ by transforming its coefficients by $\tilde{\boldsymbol{v}} = \boldsymbol{W}\boldsymbol{v}$. This is because the coefficients w_j are multiplied by the number '0' augmenting the column $\boldsymbol{v} = (v_j)$. Indeed, the vector $\mathbf{v} = \underrightarrow{PQ}$ is not changed when the whole space is mapped onto itself by a translation.

1.2.2.4. The geometric meaning of (W, w)

Given the matrix–column pair ($\boldsymbol{W}$, $\boldsymbol{w}$) of a symmetry operation W, the geometric interpretation of W, *i.e.* the type of operation, screw or glide component, location *etc.*, can be calculated provided the coordinate system to which ($\boldsymbol{W}$, $\boldsymbol{w}$) refers is known.

(1) Evaluation of the matrix part $\boldsymbol{W}$:

(*a*) *Type of operation*: In general the coefficients of the matrix depend on the choice of the basis; a change of basis changes the coefficients, see Section 1.5.2. However, there are geometric quantities that are independent of the basis.

(i) The preservation of the handedness of a chiral object, *i.e.* the question of whether the symmetry operation is a rotation or rotoinversion, is a geometric property which is deduced from the determinant of $\boldsymbol{W}$: $\det(\boldsymbol{W}) = +1$: *rotation*; $\det(\boldsymbol{W}) = -1$: *rotoinversion*.

(ii) The *angle of rotation* ϕ. This does not depend on the coordinate basis. The corresponding invariant of the matrix $\boldsymbol{W}$ is the trace and it is defined by $tr(\boldsymbol{W}) = W_{11} + W_{22} + W_{33}$. The rotation angle ϕ of the rotation or of the rotation part of a rotoinversion can be calculated from the trace by the formula

$$\pm\mathrm{tr}(\boldsymbol{W}) = 1 + 2\cos\phi \quad \text{or} \quad \cos\phi = (\pm\mathrm{tr}(\boldsymbol{W}) - 1)/2. \tag{1.2.2.12}$$

The + sign is used for rotations, the − sign for rotoinversions.

The type of isometry: the types 1, 2, 3, 4, 6 or $\bar{1}$, $\bar{2} = m$, $\bar{3}$, $\bar{4}$, $\bar{6}$ can be uniquely specified by the matrix invariants: the determinant $\det(\boldsymbol{W})$ and the trace $\mathrm{tr}(\boldsymbol{W})$:

	$\det(\boldsymbol{W}) = +1$					$\det(\boldsymbol{W}) = -1$				
$\mathrm{tr}(\boldsymbol{W})$	3	2	1	0	−1	−3	−2	−1	0	1
Type	1	6	4	3	2	$\bar{1}$	$\bar{6}$	$\bar{4}$	$\bar{3}$	$\bar{2} = m$
Order	1	6	4	3	2	2	6	4	6	2

(*b*) *Rotation or rotoinversion axis*: All symmetry operations (except 1 and $\bar{1}$) have a characteristic axis (the *rotation* or *rotoinversion axis*). The direction $\boldsymbol{u}$ of this axis is invariant under the symmetry operation:

$$\pm\boldsymbol{W}\boldsymbol{u} = \boldsymbol{u} \quad \text{or} \quad (\pm\boldsymbol{W} - \boldsymbol{I})\boldsymbol{u} = \boldsymbol{o}. \tag{1.2.2.13}$$

The + sign is for rotations, the − sign for rotoinversions.

In the case of a k-fold rotation, the direction $\boldsymbol{u}$ can be calculated by the equation

$$\boldsymbol{u} = \boldsymbol{Y}(\boldsymbol{W})\boldsymbol{v} = (\boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{v}, \tag{1.2.2.14}$$

where $\boldsymbol{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$ is an arbitrary direction. The direction $\boldsymbol{Y}(\boldsymbol{W})\boldsymbol{v}$ is invariant under the symmetry operation $\boldsymbol{W}$ as the multiplication with $\boldsymbol{W}$ just permutes the terms of $\boldsymbol{Y}$. If the application of equation (1.2.2.14) results in $\boldsymbol{u} = \boldsymbol{o}$, then the direction $\boldsymbol{v}$ is perpendicular to $\boldsymbol{u}$ and another direction $\boldsymbol{v}$ has to be selected. In the case of a rotoinversion $\boldsymbol{W}$, the direction $\boldsymbol{Y}(-\boldsymbol{W})\boldsymbol{v}$ gives the direction of the rotoinversion axis. For $\bar{2} = m$, $\boldsymbol{Y}(-\boldsymbol{W}) = -\boldsymbol{W} + \boldsymbol{I}$.

(*c*) *Sense of rotation* (for rotations or rotoinversions with $k > 2$): The sense of rotation is determined by the sign of the determinant of the matrix $\boldsymbol{Z}$, given by $\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det\boldsymbol{W})\boldsymbol{W}\boldsymbol{x}]$, where $\boldsymbol{u}$ is the vector of equation (1.2.2.14) and $\boldsymbol{x}$ is a non-parallel vector of $\boldsymbol{u}$, *e.g.* one of the basis vectors.

Examples are given later.

(2) Analysis of the translation column $\boldsymbol{w}$:

(*a*) If $\boldsymbol{W}$ is the matrix of a rotation of order k or of a reflection ($k = 2$), then $\boldsymbol{W}^k = \boldsymbol{I}$, and one determines the *intrinsic translation part* (or *screw part* or *glide part*) of the symmetry operation, also called the *intrinsic translation component* of the symmetry operation, $\boldsymbol{w}_g = \boldsymbol{t}/k$ by

$$(\boldsymbol{W}, \boldsymbol{w})^k = (\boldsymbol{W}^k, \boldsymbol{W}^{k-1}\boldsymbol{w} + \boldsymbol{W}^{k-2}\boldsymbol{w} + \ldots + \boldsymbol{W}\boldsymbol{w} + \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{t}) \quad (1.2.2.15)$$

or

$$\boldsymbol{w}_g = \boldsymbol{t}/k = \frac{1}{k}(\boldsymbol{W}^{k-1} + \boldsymbol{W}^{k-2} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} = \frac{1}{k}\boldsymbol{Y}(\boldsymbol{W})\,\boldsymbol{w}. \quad (1.2.2.16)$$

The vector with the column of coefficients $\boldsymbol{w}_g = \boldsymbol{t}/k$ is called the *screw* or *glide vector*. This vector is invariant under the symmetry operation: $\boldsymbol{W}\boldsymbol{w}_g = \boldsymbol{w}_g$. Indeed, multiplication with $\boldsymbol{W}$ permutes only the terms on the right side of equation (1.2.2.16). Thus, the screw vector of a screw rotation is parallel to the screw axis. The glide vector of a glide reflection is left invariant for the same reason. It is parallel to the glide plane because $(-\boldsymbol{W} + \boldsymbol{I})(\boldsymbol{I} + \boldsymbol{W}) = \boldsymbol{O}$.

If $\boldsymbol{t} = \boldsymbol{o}$ holds, then $(\boldsymbol{W}, \boldsymbol{w})$ describes a *rotation* or *reflection*. For $\boldsymbol{t} \neq \boldsymbol{o}$, $(\boldsymbol{W}, \boldsymbol{w})$ describes a *screw rotation* or *glide reflection*. One forms the so-called *reduced operation* by subtracting the *intrinsic translation part* $\boldsymbol{w}_g = \boldsymbol{t}/k$ from $(\boldsymbol{W}, \boldsymbol{w})$:

$$(\boldsymbol{I}, -\boldsymbol{t}/k)(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} - \boldsymbol{w}_g) = (\boldsymbol{W}, \boldsymbol{w}_l). \quad (1.2.2.17)$$

The column $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{t}/k$ is called the *location part* (or the *location component* of the translation part) of the symmetry operation because it determines the position of the rotation or screw–rotation axis or of the reflection or glide–reflection plane in space.

(*b*) The set of *fixed points* of a symmetry operation is obtained by solving the equation

$$\boldsymbol{W}\boldsymbol{x}_F + \boldsymbol{w} = \boldsymbol{x}_F. \quad (1.2.2.18)$$

Equation (1.2.2.18) has a unique solution for all roto-inversions (including $\bar{1}$, excluding $\bar{2} = m$). There is a one-dimensional set of solutions for rotations (the rotation axis) and a two-dimensional set of solutions for reflections (the mirror plane). For translations, screw rotations and glide reflections, there are no solutions: there are no fixed points. However, a solution is found for the reduced operation, *i.e.* after subtraction of the intrinsic translation part, *cf.* equation (1.2.2.17)

$$\boldsymbol{W}\boldsymbol{x}_F + \boldsymbol{w}_l = \boldsymbol{x}_F. \quad (1.2.2.19)$$

(Note that the reduced operation of a translation is the identity, whose set of fixed points is the whole space.)

The formulae of this section enable the user to find the geometric contents of any symmetry operation. In practice, the geometric meanings for all symmetry operations which are listed in the *General position* blocks of the space-group tables of Part 2 can be found in the corresponding **Symmetry operations** blocks of the space-group tables. The explanation of the symbols for the symmetry operations is found in Sections 1.4.2 and 2.1.3.9.

The procedure for the geometric interpretation of the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ of the symmetry operations is illustrated by three examples of the space group $Ia\bar{3}d$, No. 230 (*cf.* the space-group tables of Chapter 2.3).

Examples

(1) Consider the symmetry operation $y + \frac{1}{4}, \bar{x} + \frac{1}{4}, z + \frac{3}{4}$ [symmetry operation (15) of the *General position* (0, 0, 0) block of the space group $Ia\bar{3}d$]. Its matrix–column pair is given by

$$\boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \boldsymbol{w} = \begin{pmatrix} 1/4 \\ 1/4 \\ 3/4 \end{pmatrix}.$$

Type of operation: the values of $\det(\boldsymbol{W}) = 1$ and $\mathrm{tr}(\boldsymbol{W}) = 1$ show that the symmetry operation is a fourfold rotation.
The direction of rotation axis $\boldsymbol{u}$: The application of equation (1.2.2.14) with the matrix

$$\boldsymbol{Y}(\boldsymbol{W}) = (\boldsymbol{W}^3 + \boldsymbol{W}^2 + \boldsymbol{W} + \boldsymbol{I}) = \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

yields the direction $\boldsymbol{u} = [001]$ of the fourfold rotation axis.
Sense of rotation: The negative sense of rotation follows from $\det(\boldsymbol{Z}) = -1$, where the matrix

$$\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\boldsymbol{W}\boldsymbol{x}] = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$$

(here, $\boldsymbol{x} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ is taken as a vector non-parallel to $\boldsymbol{u}$).

Screw component: The intrinsic translation part (screw component) $\boldsymbol{w}_g$ of the symmetry operation is calculated from

$$\boldsymbol{w}_g = \tfrac{1}{4}\boldsymbol{Y}(\boldsymbol{W})\boldsymbol{w} = 1/4\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}\begin{pmatrix} 1/4 \\ 1/4 \\ 3/4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 3/4 \end{pmatrix}.$$

Location of the symmetry operation: The location of the fourfold screw rotation is given by the fixed points of the reduced symmetry operation $(\boldsymbol{W}, \boldsymbol{w} - \boldsymbol{w}_g)$. The set of fixed points $\boldsymbol{x}_F = \begin{pmatrix} 1/4 \\ 0 \\ z \end{pmatrix}$ is obtained from the equation

$$\begin{pmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} + \begin{pmatrix} 1/4 \\ 1/4 \\ 0 \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}.$$

Following the conventions for the designation of symmetry operations adopted in this volume (*cf.* Section 1.4.2 and 2.1.3.9), the symbol of the symmetry operation $y + \frac{1}{4}$, $-x + \frac{1}{4}$, $z + \frac{3}{4}$ is given by $4^-(0, 0, \frac{3}{4})\ \ \frac{1}{4}, 0, z$.

(2) The symmetry operation $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y$ with

$$\boldsymbol{W} = \begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \boldsymbol{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$$

corresponds to the entry No. (30) of the *General position* (0, 0, 0) block of the space group $Ia\bar{3}d$, No. 230.

Type of operation: the values of $\det(\boldsymbol{W}) = -1$ and $\mathrm{tr}(\boldsymbol{W}) = 0$ show that symmetry operation is a threefold rotoinversion.

The direction of rotoinversion axis $\boldsymbol{u}$:

$$\begin{aligned}\boldsymbol{Y}(-\boldsymbol{W}) &= (\boldsymbol{W}^2 - \boldsymbol{W} + \boldsymbol{I}) \\ &= \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right) \\ &= \begin{pmatrix} 1 & \bar{1} & 1 \\ \bar{1} & 1 & \bar{1} \\ 1 & \bar{1} & 1 \end{pmatrix}\end{aligned}$$

yields the direction $\boldsymbol{u} = [\bar{1}1\bar{1}]$ from $\boldsymbol{v} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$.

Sense of rotation: The positive sense of rotation follows from the positive sign of the determinant of the matrix $\boldsymbol{Z}$, $\det(\boldsymbol{Z}) = 1$, where the matrix

$$\boldsymbol{Z} = [\boldsymbol{u}|\boldsymbol{x}|(\det \boldsymbol{W})\boldsymbol{W}\boldsymbol{x}] = \begin{pmatrix} \bar{1} & 0 & 1 \\ 1 & 0 & 0 \\ \bar{1} & 1 & 0 \end{pmatrix}$$

(here, $\boldsymbol{x} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ is taken as a vector non-parallel to $\boldsymbol{u}$).

Location of the symmetry operation: The solution $x_F = 0$, $y_F = 1/2$, $z_F = 1/2$ of the fixed-point equation of the rotoinversion

$$\begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}$$

gives the coordinates of the inversion centre on the rotoinversion axis. An obvious description of a line along the direction $\boldsymbol{u} = [\bar{1}1\bar{1}]$ and passing through the point $(0, 1/2, 1/2)$ is given by the parametric expression $\bar{u}, u + 1/2, \bar{u} + 1/2$. The choice of the free parameter $u = x + 1/2$ results in the description $\bar{x} - 1/2, x + 1, \bar{x}$ of the rotoinversion axis found in the **Symmetry operation** (0, 0, 0) block. The convention adopted in this volume to have zero constant at the z coordinate of the description of the $\bar{3}$ axis determines the specific choice of the free parameter.

The geometric characteristics of the symmetry operation $\bar{z} + \frac{1}{2}, x + \frac{1}{2}, y$ are reflected in its symbol $\bar{3}^+\ \bar{x} - 1/2, x + 1, \bar{x};\ 0, \frac{1}{2}, \frac{1}{2}$.

(3) The matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ of the symmetry operation (37) $\bar{y} + 3/4, \bar{x} + 1/4, z + 1/4$ of the *General position* $(1/2, 1/2, 1/2)$ block of the space group $Ia\bar{3}d$ is given by

$$\boldsymbol{W} = \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \boldsymbol{w} = \begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix}.$$

Type of operation: The values of the determinant $\det(\boldsymbol{W}) = -1$ and the trace $\mathrm{tr}(\boldsymbol{W}) = +1$ indicate that the symmetry operation is a reflection.

Normal $\boldsymbol{u}$ *of the reflection plane*: The orientation of the reflection plane in space is determined by its normal $\boldsymbol{u}$, which is directed along [110]. The direction of $\boldsymbol{u}$ follows from the matrix equation

$$\begin{aligned}\boldsymbol{u} &= (-\boldsymbol{W} + \boldsymbol{I})\boldsymbol{v} \\ &= \left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)\boldsymbol{v} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}\boldsymbol{v},\end{aligned}$$

where $\boldsymbol{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$ is arbitrary.

Glide component: The glide component $\boldsymbol{w}_g = \begin{pmatrix} 1/4 \\ -1/4 \\ 1/4 \end{pmatrix}$, determined from the equation

$$\begin{aligned}\boldsymbol{w}_g &= \tfrac{1}{2}(\boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} \\ &= \tfrac{1}{2}\left(\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)\begin{pmatrix} 3/4 \\ 1/4 \\ 1/4 \end{pmatrix},\end{aligned}$$

indicates that the symmetry operation is a *d*-glide reflection. As expected, the translation vector

$$\mathbf{t} = 2\boldsymbol{w}_g = \begin{pmatrix} 1/2 \\ -1/2 \\ 1/2 \end{pmatrix}$$

corresponds to a centring translation.

Location of the symmetry operation: The location of the *d*-glide plane follows from the set of fixed points (x_F, y_F, z_F) of the reduced symmetry operation

$$(\boldsymbol{W}, \boldsymbol{w} - \boldsymbol{w}_g) = \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 3/4 - 1/4 \\ 1/4 - (-1/4) \\ 1/4 - 1/4 \end{pmatrix}\right):$$

$$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} + \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}.$$

Thus, the set of fixed points (the *d*-glide plane) can be described as $x + 1/2, \bar{x}, z$.

The symbol $d\,(1/4, -1/4, 1/4)\ x + 1/2, \bar{x}, z$ of the symmetry operation (37) $\bar{y} + 3/4, \bar{x} + 1/4, z + 1/4$, found in the **Symmetry operations** $(1/2, 1/2, 1/2)$ block of the space-group table of $Ia\bar{3}d$ in Chapter 2.3, comprises the essential geometric characteristics of the symmetry operation, *i.e.* its type, glide component and location. It is worth repeating that according to the conventions adopted in the space-group tables of Part 2, the mirror planes are specified by their sets of fixed points and not by the normals to the planes (*cf.* Section 1.4.2 for more details).

1.2.2.5. Determination of matrix–column pairs of symmetry operations

The specification of the symmetry operations by their types, screw or glide components and locations is sufficient to determine the corresponding matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$. The general idea is to determine the image points $\widetilde{X}$ of some points X under the symmetry operation by applying geometrical considerations. The 12 unknown coefficients of $(\boldsymbol{W}, \boldsymbol{w})$ (nine coefficients W_{ik} and three coefficients w_j) can then be calculated as solutions of 12 inhomogeneous linear equations obtained from the system of

equations (1.2.2.1) written for four pairs (point → image point), provided the points X are linearly independent. In fact, because of the special form of the matrix–column pairs, in many cases it is possible to reduce and simplify considerably the calculations necessary for the determination of $(\boldsymbol{W}, \boldsymbol{w})$: the determination of the image points of the origin O and of the three 'coordinate points' A (1, 0, 0), B (0, 1, 0) and C (0, 0, 1) under the symmetry operation is sufficient for the determination of its matrix–column pair.

(1) *The origin*: Let $\widetilde{O}$ with coordinates $\tilde{\boldsymbol{o}}$ be the image of the origin O with coordinates $\boldsymbol{o}$, *i.e.* $x_\circ = y_\circ = z_\circ = 0$. Examination of the equations (1.2.2.1) shows that $\tilde{\boldsymbol{o}} = \boldsymbol{w}$, *i.e.* the column $\boldsymbol{w}$ can be determined separately from the coefficients of the matrix $\boldsymbol{W}$.

(2) *The coordinate points*: We consider the point A. Inserting $x = 1, \quad y = z = 0$ in equations (1.2.2.1) one obtains $\tilde{x}_i = W_{i1} + w_i$ or $W_{i1} = \tilde{x}_i - w_i, i = 1, 2, 3$. The first column of $\boldsymbol{W}$ is separated from the others, and for the solution only the known coefficients w_i have to be subtracted from the coordinates $\tilde{x}_i$ of the image point $\tilde{A}$ of A. Analogously one calculates the coefficients W_{i2} from the image of point B (0, 1, 0) and W_{i3} from the image of point C (0, 0, 1).

Example

What is the pair $(\boldsymbol{W}, \boldsymbol{w})$ for a glide reflection with the plane through the origin, the normal of the glide plane parallel to **c**, and with the glide vector $\boldsymbol{w}_g = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$?

(*a*) *Image of the origin O*: The origin is left invariant by the reflection part of the mapping; it is shifted by the glide part to 1/2, 1/2, 0 which are the coordinates of $\tilde{O}$. Therefore, $\boldsymbol{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}$.

(*b*) *Images of the coordinate points*. Neither of the points A and B are affected by the reflection part, but A is then shifted to 3/2, 1/2, 0 and B to 1/2, 3/2, 0. This results in the equations $3/2 = W_{11} + 1/2, \quad 1/2 = W_{21} + 1/2, \quad 0 = W_{31} + 0$ for A and $1/2 = W_{12} + 1/2, 3/2 = W_{22} + 1/2, \quad 0 = W_{32} + 0$ for B.

One obtains $W_{11} = 1, W_{21} = W_{31} = W_{12} = 0, W_{22} = 1$ and $W_{32} = 0$. Point C: 0, 0, 1 is reflected to 0, 0, −1 and then shifted to 1/2, 1/2, −1.

This means $1/2 = W_{13} + 1/2, \quad 1/2 = W_{23} + 1/2, \quad -1 = W_{33} + 0$ or $W_{13} = W_{23} = 0, W_{33} = -1$.

(*c*) *The matrix–column pair* is thus

$$\boldsymbol{W} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \text{ and } \boldsymbol{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix},$$

which can be represented by the coordinate triplet $x + 1/2, y + 1/2, \bar{z}$ [*cf.* Section 1.2.2.1.1 for the shorthand notation of $(\boldsymbol{W}, \boldsymbol{w})$].

The problem of the determination of $(\boldsymbol{W}, \boldsymbol{w})$ discussed above is simplified if it is reduced to the special case of the derivation of matrix–column pairs of space-group symmetry operations (*General position* block) from their symbols (**Symmetry operations** block) found in the space-group tables of Part 2 of this volume. The main simplification comes from the fact that for all symmetry operations of space groups, the rotation parts $\boldsymbol{W}$ referring to conventional coordinate systems are known and listed in Tables 1.2.2.1 and 1.2.2.2. In this way, given the symbol of the symmetry operation and using the tabulated data, one can write down directly the corresponding rotation part $\boldsymbol{W}$.

The translation part $\boldsymbol{w}$ of the symmetry operation has two components: $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$. The *intrinsic translation part* (or screw or glide component) is given explicitly in the symmetry operation symbol. The *location part* $\boldsymbol{w}_l$ of $\boldsymbol{w}$ is derived from the equations

$$(\boldsymbol{W}, \boldsymbol{w}_l)\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}, \text{ i.e. } \boldsymbol{w}_l = (\boldsymbol{I} - \boldsymbol{W})\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix}. \quad (1.2.2.20)$$

Here, (x_F, y_F, z_F) are the coordinates of an arbitrary fixed point of the symmetry operation.

Example

Consider the symbol $3^-(1/3, 1/3, -1/3)\ \ \bar{x} + 1/3, \bar{x} + 1/6, x$ of the symmetry operation No. (11) of the **Symmetry operations** (0, 0, 0) block of the space group $Ia\bar{3}d$ (230). The corresponding rotational part $\boldsymbol{W}$ is read directly from Table 1.2.2.1:

$$\boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}.$$

The location part $\boldsymbol{w}_l$ is determined by the matrix equations

$$\boldsymbol{w}_l = \left(\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}\right)\begin{pmatrix} 1/3 \\ 1/6 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/6 \\ 1/6 \\ 1/3 \end{pmatrix}$$

[*cf.* Equation (1.2.2.20)]. The point with coordinates $x_F = 1/3, \quad y_F = 1/6, \quad z_F = 0$ is on the screw axis of $3^- \ \ \bar{x} + 1/3, \bar{x} + 1/6, x$, *i.e.* one of the fixed points of the reduced symmetry operation $(\boldsymbol{W}, \boldsymbol{w}_l)$. The translation part $\boldsymbol{w}$ of the matrix–column pair of the symmetry operation is given by

$$\boldsymbol{w} = \boldsymbol{w}_l + \boldsymbol{w}_g = \begin{pmatrix} 1/6 \\ 1/6 \\ 1/3 \end{pmatrix} + \begin{pmatrix} 1/3 \\ 1/3 \\ -1/3 \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}.$$

The coordinate triplet $y + 1/2, \bar{z} + 1/2, \bar{x}$, corresponding to the derived matrix–column pair

$$(\boldsymbol{W}, \boldsymbol{w}) = \left(\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 0 \end{pmatrix}\right),$$

coincides exactly with the coordinate triplet listed under No. (11) in the (0, 0, 0) block of the *General positions* of the space group $Ia\bar{3}d$.

1.2.3. Symmetry elements

In the 1970s, when the International Union of Crystallography (IUCr) planned a new series of *International Tables for Crystallography* to replace the series *International Tables for X-ray Crystallography* (1952), there was some confusion about the use of the term *symmetry element*. Crystallographers and mineralogists had used this term for rotation and rotoinversion axes and reflection planes, in particular for the description of the morphology of crystals, for a long time, although there had been no strict definition of 'symmetry element'. With the impact of mathematical group theory in crystallography the term *element* was introduced with another meaning, in which an element is a member of a set, in particular as a group element of a group.

Table 1.2.3.1
Symmetry elements in point and space groups

Name of symmetry element	Geometric element	Defining operation (d.o.)	Operations in element set
Mirror plane	Plane p	Reflection through p	D.o. and its coplanar equivalents†
Glide plane	Plane p	Glide reflection through p; $2\mathbf{v}$ (not $\mathbf{v}$) a lattice-translation vector	D.o. and its coplanar equivalents†
Rotation axis	Line l	Rotation around l, angle $2\pi/N$, N = 2, 3, 4 or 6	1st ... $(N-1)$th powers of d.o. and their coaxial equivalents‡
Screw axis	Line l	Screw rotation around l, angle $2\pi/N$, $u = j/N$ times shortest lattice translation along l, right-hand screw, N = 2, 3, 4 or 6, j = 1, ..., $(N-1)$	1st ... $(N-1)$th powers of d.o. and their coaxial equivalents‡
Rotoinversion axis	Line l and point P on l	Rotoinversion: rotation around l, angle $2\pi/N$, followed by inversion through P, N = 3, 4 or 6	D.o. and its inverse
Centre	Point P	Inversion through P	D.o. only

† That is, all glide reflections through the same reflection plane, with glide vectors $\mathbf{v}$ differing from that of the d.o. (taken to be zero for reflections) by a lattice-translation vector. The glide planes a, b, c, n, d and e are distinguished (*cf.* Table 2.1.2.1). ‡ That is, all rotations and screw rotations around the same axis l, with the same angle and sense of rotation and the same screw vector $\mathbf{u}$ (zero for rotation) up to a lattice-translation vector.

In crystallography these group elements, however, were the symmetry operations of the symmetry groups, not the crystallographic symmetry elements. Therefore, the IUCr Commission on Crystallographic Nomenclature appointed an *Ad-hoc* Committee on the Nomenclature of Symmetry with P. M. de Wolff as Chairman to propose definitions for terms of crystallographic symmetry and for several classifications of crystallographic space groups and point groups.

In the reports of the *Ad-hoc* Committee, de Wolff *et al.* (1989) and (1992) with *Addenda*, Flack *et al.* (2000), the results were published. To define the term *symmetry element* for any symmetry operation was more complicated than had been envisaged previously, in particular for unusual screw and glide components.

According to the proposals of the Committee the following procedure has been adopted (*cf.* also Table 1.2.3.1):

(1) No symmetry element is defined for the identity and the (lattice) translations.

(2) For any symmetry operation of point groups and space groups with the exception of the rotoinversions $\bar{3}$, $\bar{4}$ and $\bar{6}$, the *geometric element* is defined as the *set of fixed points* (the second column of Table 1.2.3.1) of the *reduced operation*, *cf.* equation (1.2.2.17). For reflections and glide reflections this is a plane; for rotations and screw rotations it is a line, for the inversion it is a point. For the rotoinversions $\bar{3}$, $\bar{4}$ and $\bar{6}$ the geometric element is a line with a point (the inversion centre) on this line.

(3) The *element set* (*cf.* the last column of Table 1.2.3.1) is defined as a set of operations that share the same geometric element. The element set can consist of symmetry operations of the same type (such as the powers of a rotation) or of different types, *e.g.* by a reflection and a glide reflection through the same plane. The *defining operation* (d.o.) may be any symmetry operation from the element set that suffices to identify the symmetry element. In most cases, the 'simplest' symmetry operation from the element set is chosen as the d.o. (*cf.* the third column of Table 1.2.3.1). For reflections and glide reflections the element set includes the defining operation and all glide reflections through the same reflection plane but with glide vectors differing by a lattice-translation vector, *i.e.* the so-called *coplanar equivalents*. For rotations and screw rotations of angle $2\pi/k$ the element set is the defining operation, its 1st ... $(k-1)$th powers and all rotations and screw rotations with screw vectors differing from that of the defining operation by a lattice-translation vector, known as *coaxial equivalents*. For a rotoinversion the element set includes the defining operation and its inverse.

(4) The combination of the geometric element and its element set is indicated by the name *symmetry element*. The names of the symmetry elements (first column of Table 1.2.3.1) are combinations of the name of the defining operation attached to the name of the corresponding geometric element. Names of symmetry elements are *mirror plane*, *glide plane*, *rotation axis*, *screw axis*, *rotoinversion axis* and *centre*.[2] This allows such statements as *this point lies on a rotation axis* or *these operations belong to a glide plane*.

Examples

(1) *Glide and mirror planes*. The element set of a glide plane with a glide vector $\mathbf{v}$ consists of infinitely many different glide reflections with glide vectors that are obtained from $\mathbf{v}$ by adding any lattice-translation vector parallel to the glide plane, including centring translations of centred cells.

(a) It is important to note that if among the infinitely many glide reflections of the element set of the same plane there exists one operation with zero glide vector, then this operation is taken as the *defining operation* (d.o). Consider, for example, the symmetry operation $x+1/2,\ y+1/2,\ -z+1/2$ of *Cmcm* (63) [*General position* $(1/2, 1/2, 0)$ block]. This is an n-glide reflection through the plane $x, y, 1/4$. However, the corresponding symmetry element is a mirror plane, as among the glide reflections of the element set of the plane $x, y, 1/4$ one finds the reflection $x, y, -z+1/2$ [symmetry operation (6) of the *General position* $(0, 0, 0)$ block].

(b) The symmetry operation $x+5/2, y-7/2, -z+3$ is a glide reflection. Its geometric element is the plane $x, y, 3/2$. Its symmetry element is a glide plane in space group *Pmmn* (59) because there is no lattice translation by which the glide vector can be changed to $\mathbf{o}$. If, however, the same mapping is a symmetry operation of space group *Cmmm* (65), then its symmetry element is a reflection plane because the glide vector with components $5/2, -7/2, 0$ can be cancelled through a translation $(2+\frac{1}{2})\mathbf{a}+(-4+\frac{1}{2})\mathbf{b}$, which is a lattice translation in a C lattice. Evidently, the correct specification of the symmetry element is possible only with respect to a specific translation lattice.

[2] The proposal to introduce the symbols for the symmetry elements Em, Eg, En, En_j, $E\bar{n}$ and $E\bar{1}$ was not taken up in practice. The printed and graphical symbols of symmetry elements used throughout the space-group tables of Part 2 are introduced in Section 2.1.2 and listed in Tables 2.1.2.1 to 2.1.2.7.

(*c*) Similarly, in *Cmme* (67) with an *a*-glide reflection $x+1/2, y, \overline{z}$, the *b*-glide reflection $x, y+1/2, \overline{z}$ also occurs. The geometric element is the plane $x, y, 0$ and the symmetry element is an *e*-glide plane.

In fact, all vectors $(u+\frac{1}{2})\mathbf{a}+v\mathbf{b}+\frac{1}{2}k(\mathbf{a}+\mathbf{b})$, u, v, k integers, are glide vectors of glide reflections through the (001) plane of a space group with a *C*-centred lattice. Among them one finds a glide reflection *b* with a glide vector $\frac{1}{2}\mathbf{b}$ related to $\frac{1}{2}\mathbf{a}$ by the centring translation; an *a*-glide reflection and a *b*-glide reflection share the same plane as a geometric element. Their symmetry element is thus an *e*-glide plane.

(*d*) In general, the *e*-glide planes are symmetry elements characterized by the existence of two glide reflections through the same plane with perpendicular glide vectors and with the additional requirement that at least one glide vector is along a crystal axis (de Wolff *et al.*, 1992). The *e*-glide designation of glide planes occurs only when a centred cell represents the choice of basis (*cf.* Table 2.1.2.2). The 'double' *e*-glide planes are indicated by special graphical symbols on the symmetry-element diagrams of the space groups (*cf.* Tables 2.1.2.3 and 2.1.2.4). For example, consider the space group *I*4*cm* (108). The symmetry operations (8) $y, x, z+1/2$ [*General position* (0, 0, 0) block] and (8) $y+1/2, x+1/2, z$ [*General position* (1/2, 1/2, 1/2) block] are glide reflections through the same x, x, z plane, and their glide vectors $\frac{1}{2}\mathbf{c}$ and $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ are related by the centring $(1/2, 1/2, 1/2)$ translation. The corresponding symmetry element is an *e*-glide plane and it is easily recognized on the symmetry-element diagram of *I*4*cm* shown in Chapter 2.3.

(2) *Screw and rotation axes*. The element set of a screw axis is formed by a screw rotation of angle $2\pi/N$ with a screw vector **u**, its $(N-1)$ powers and all its co-axial equivalents, *i.e.* screw rotations around the same axis, with the same angle and sense of rotation, with screw vectors obtained by adding a lattice-translation vector parallel to **u**.

(*a*) Twofold screw axis $\parallel$ [001] in a primitive cell: the element set is formed by all twofold screw rotations around the same axis with screw vectors of the type $(u+\frac{1}{2})\mathbf{c}$, *i.e.* screw components as $\frac{1}{2}\mathbf{c}$, $-\frac{1}{2}\mathbf{c}$, $\frac{3}{2}\mathbf{c}$ *etc*.

(*b*) The symmetry operation $4-x, -2-y, z+5/2$ is a screw rotation of space group $P222_1$ (17). Its geometric element is the line $2, -1, z$ and its symmetry element is a screw axis.

(*c*) The determination of the complete element set of a geometric element is important for the correct designation of the corresponding symmetry element. For example, the symmetry element of a twofold screw rotation with an axis through the origin is a twofold screw axis in the space group $P222_1$ but a fourfold screw axis in $P4_1$ (76).

(3) *Special case*. In point groups $6/m$, $6/mmm$ and space groups $P6/m$ (175), $P6/mmm$ (191) and $P6/mcc$ (192) the geometric elements of the defining operations $\overline{6}$ and $\overline{3}$ are the same. To make the element sets unique, the geometric elements should not be given just by a line and a point on it, but should be labelled by these operations. Then the element sets and thus the symmetry element are unique (Flack *et al.*, 2000).

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1.3. A general introduction to space groups

B. Souvignier

1.3.1. Introduction

We recall from Chapter 1.2 that an *isometry* is a mapping of the point space $\mathbb{E}^n$ which preserves distances and angles. From the mathematical viewpoint, $\mathbb{E}^n$ is an *affine space* in which two points differ by a unique vector in the underlying *vector space* $\mathbb{V}^n$. The crucial difference between these two types of spaces is that in an affine space no point is distinguished, whereas in a vector space the zero vector plays a special role, namely as the identity element for the addition of vectors. After choosing an origin O, the points of the affine space $\mathbb{E}^n$ are in one-to-one correspondence with the vectors of $\mathbb{V}^n$ by identifying a point P with the difference vector $\overrightarrow{OP}$.

A *crystallographic space-group operation* is an isometry that maps a crystal pattern onto itself. Since isometries are invertible and the composition of two isometries leaves a crystal pattern invariant as a whole if the two single isometries do so, the space-group operations form a group $\mathcal{G}$, called a *crystallographic space group*.

As a mapping of points in an affine space, a space-group operation is an affine mapping and is thus composed of a linear mapping of the underlying vector space and a translation. Once a coordinate system has been chosen, space-group operations are conveniently represented as *matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$, where $\boldsymbol{W}$ is the *linear part* and $\boldsymbol{w}$ the *translation part* and a point with coordinates $\boldsymbol{x}$ is mapped to $\boldsymbol{Wx} + \boldsymbol{w}$ (*cf.* Section 1.2.2).

A translation is a matrix–column pair of the form $(\boldsymbol{I}, \boldsymbol{w})$, where $\boldsymbol{I}$ is the unit matrix and all translations taken together form the *translation subgroup* $\mathcal{T}$ of $\mathcal{G}$. The translation subgroup is an infinite group that forms an abelian normal subgroup of $\mathcal{G}$. The factor group $\mathcal{G}/\mathcal{T}$ is a finite group that can be identified with the group of linear parts of $\mathcal{G}$ *via* the mapping $(\boldsymbol{W}, \boldsymbol{w}) \mapsto \boldsymbol{W}$, which simply forgets about the translation part. The group $\mathcal{P} = \{\boldsymbol{W} \mid (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}\}$ of linear parts occurring in $\mathcal{G}$ is called the *point group* $\mathcal{P}$ of $\mathcal{G}$.

The representation of space-group operations as matrix–column pairs is clearly adapted to the fact that space groups can be built from these two parts, the translation subgroup and the point group. This viewpoint will be discussed in detail in Section 1.3.3. It allows one to treat space groups in many aspects analogously to finite groups, although, due to the infinite translation subgroup, they are of course infinite groups.

1.3.2. Lattices

A crystal pattern is defined to be periodic in three linearly independent directions, which means that it is invariant under translations in three linearly independent directions. This periodicity implies that the crystal pattern extends infinitely in all directions. Since the atoms of a crystal form a discrete pattern in which two different points have a certain minimal distance, the translations that fix the crystal pattern as a whole cannot have arbitrarily small lengths. If $\mathbf{v}$ is a vector such that the crystal pattern is invariant under a translation by $\mathbf{v}$, the periodicity implies that the pattern is invariant under a translation by $m\mathbf{v}$ for every integer m. Furthermore, if a crystal pattern is invariant under translations by $\mathbf{v}$ and $\mathbf{w}$, it is also invariant by the composition of these two translations, which is the translation by $\mathbf{v} + \mathbf{w}$. This shows that the set of vectors by which the translations in a space group move the crystal pattern is closed under taking integral linear combinations. This property is formalized by the mathematical concept of a *lattice* and the translation subgroups of space groups are best understood by studying their corresponding lattices. These lattices capture the periodic nature of the underlying crystal patterns and reflect their geometric properties.

1.3.2.1. Basic properties of lattices

The two-dimensional vector space $\mathbb{V}^2$ is the space of columns $\begin{pmatrix} x \\ y \end{pmatrix}$ with two real components $x, y \in \mathbb{R}$ and the three-dimensional vector space $\mathbb{V}^3$ is the space of columns $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ with three real components $x, y, z \in \mathbb{R}$. Analogously, the n-dimensional vector space $\mathbb{V}^n$ is the space of columns $\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}$ with n real components.

For the sake of clarity we will restrict our discussions to three-dimensional (and occasionally two-dimensional) space. The generalization to n-dimensional space is straightforward and only requires dealing with columns of n instead of three components and with bases consisting of n instead of three basis vectors.

Definition

For vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ forming a basis of the three-dimensional vector space $\mathbb{V}^3$, the set

$$\mathbf{L} := \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$$

of all *integral* linear combinations of $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *lattice* in $\mathbb{V}^3$ and the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are called a *lattice basis* of $\mathbf{L}$.

It is inherent in the definition of a crystal pattern that the translation vectors of the translations leaving the pattern invariant are closed under taking integral linear combinations. Since the crystal pattern is assumed to be discrete, it follows that all translation vectors can be written as integral linear combinations of a finite generating set. The fundamental theorem on finitely generated abelian groups (see *e.g.* Chapter 21 in Armstrong, 1997) asserts that in this situation a set of three translation vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ can be found such that all translation vectors are integral linear combinations of these three vectors. This shows that the translation vectors of a crystal pattern form a lattice with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ in the sense of the definition above.

By definition, a lattice is determined by a lattice basis. Note, however, that every two- or three-dimensional lattice has infinitely many bases.

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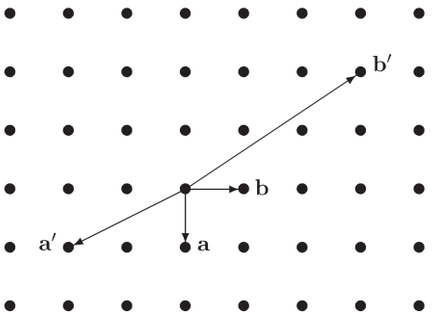

Figure 1.3.2.1
Conventional basis **a**, **b** and a non-conventional basis **a**′, **b**′ for the square lattice.

Example

The square lattice

$$\mathbf{L} = \mathbb{Z}^2 = \left\{ \begin{pmatrix} m \\ n \end{pmatrix} \mid m, n \in \mathbb{Z} \right\}$$

in $\mathbb{V}^2$ has the vectors

$$\mathbf{a} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

as its standard lattice basis. But

$$\mathbf{a}' = \begin{pmatrix} 1 \\ -2 \end{pmatrix}, \quad \mathbf{b}' = \begin{pmatrix} -2 \\ 3 \end{pmatrix}$$

is also a lattice basis of **L**: on the one hand **a**′ and **b**′ are integral linear combinations of **a**, **b** and are thus contained in **L**. On the other hand

$$-3\mathbf{a}' - 2\mathbf{b}' = \begin{pmatrix} -3 \\ 6 \end{pmatrix} + \begin{pmatrix} 4 \\ -6 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathbf{a}$$

and

$$-2\mathbf{a}' - \mathbf{b}' = \begin{pmatrix} -2 \\ 4 \end{pmatrix} + \begin{pmatrix} 2 \\ -3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \mathbf{b},$$

hence **a** and **b** are also integral linear combinations of **a**′, **b**′ and thus the two bases **a**, **b** and **a**′, **b**′ both span the same lattice (see Fig. 1.3.2.1).

The example indicates how the different lattice bases of a lattice **L** can be described. Recall that for a vector $\mathbf{v} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$ the coefficients x, y, z are called the *coordinates* and the vector $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ is called the *coordinate column* of **v** with respect to the basis **a**, **b**, **c**. The coordinate columns of the vectors in **L** with respect to a lattice basis are therefore simply columns with three integral components. In particular, if we take a second lattice basis **a**′, **b**′, **c**′ of **L**, then the coordinate columns of **a**′, **b**′, **c**′with respect to the first basis are columns of integers and thus the basis transformation $\boldsymbol{P}$ such that $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$ is an integral 3×3 matrix. But if we interchange the roles of the two bases, they are related by the inverse transformation $\boldsymbol{P}^{-1}$, *i.e.* $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (\mathbf{a}', \mathbf{b}', \mathbf{c}')\boldsymbol{P}^{-1}$, and the argument given above asserts that $\boldsymbol{P}^{-1}$ is also an integral matrix. Now, on the one hand $\det \boldsymbol{P}$ and $\det \boldsymbol{P}^{-1}$ are both integers (being determinants of integral matrices), on the other hand $\det \boldsymbol{P}^{-1} = 1/\det \boldsymbol{P}$. This is only possible if $\det \boldsymbol{P} = \pm 1$.

Summarizing, the different lattice bases of a lattice **L** are obtained by transforming a single lattice basis **a**, **b**, **c** with integral transformation matrices $\boldsymbol{P}$ such that $\det \boldsymbol{P} = \pm 1$.

1.3.2.2. Metric properties

In the three-dimensional vector space $\mathbb{V}^3$, the *norm* or *length* of a vector $\mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}$ is (due to Pythagoras' theorem) given by

$$|\mathbf{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2}.$$

From this, the *scalar product*

$$\mathbf{v} \cdot \mathbf{w} = v_x w_x + v_y w_y + v_z w_z \text{ for } \mathbf{v} = \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}, \mathbf{w} = \begin{pmatrix} w_x \\ w_y \\ w_z \end{pmatrix}$$

is derived, which allows one to express angles by

$$\cos \measuredangle(\mathbf{v}, \mathbf{w}) = \frac{\mathbf{v} \cdot \mathbf{w}}{|\mathbf{v}|\,|\mathbf{w}|}.$$

The definition of a norm function for the vectors turns $\mathbb{V}^3$ into a *Euclidean space*. A lattice **L** that is contained in $\mathbb{V}^3$ inherits the metric properties of this space. But for the lattice, these properties are most conveniently expressed with respect to a lattice basis. It is customary to choose basis vectors **a**, **b**, **c** which define a right-handed coordinate system, *i.e.* such that the matrix with columns **a**, **b**, **c** has a positive determinant.

Definition

For a lattice $\mathbf{L} \subseteq \mathbb{V}^3$ with lattice basis **a**, **b**, **c** the *metric tensor* of **L** is the 3×3 matrix

$$\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix}.$$

If $\boldsymbol{A}$ is the 3×3 matrix with the vectors **a**, **b**, **c** as its columns, then the metric tensor is obtained as the matrix product $\boldsymbol{G} = \boldsymbol{A}^{\mathrm{T}} \cdot \boldsymbol{A}$. It follows immediately that the metric tensor is a symmetric matrix, *i.e.* $\boldsymbol{G}^{\mathrm{T}} = \boldsymbol{G}$.

Example

Let

$$\mathbf{a} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

be the basis of a lattice **L**. Then the metric tensor of **L** (with respect to the given basis) is

$$\boldsymbol{G} = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

With the help of the metric tensor the scalar products of arbitrary vectors, given as linear combinations of the lattice basis, can be computed from their coordinate columns as follows: If $\mathbf{v} = x_1\mathbf{a} + y_1\mathbf{b} + z_1\mathbf{c}$ and $\mathbf{w} = x_2\mathbf{a} + y_2\mathbf{b} + z_2\mathbf{c}$, then

$$\mathbf{v}\cdot\mathbf{w} = (x_1\, y_1\, z_1)\cdot \boldsymbol{G}\cdot \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}.$$

From this it follows how the metric tensor transforms under a basis transformation $\boldsymbol{P}$. If $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$, then the metric tensor $\boldsymbol{G}'$ of $\mathbf{L}$ with respect to the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ is given by

$$\boldsymbol{G}' = \boldsymbol{P}^{\mathrm{T}}\cdot\boldsymbol{G}\cdot\boldsymbol{P}.$$

An alternative way to specify the geometry of a lattice in $\mathbb{V}^3$ is using the *cell parameters*, which are the lengths of the lattice basis vectors and the angles between them.

Definition

For a lattice $\mathbf{L}$ in $\mathbb{V}^3$ with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ the *cell parameters* (also called *lattice parameters*, *lattice constants* or *metric parameters*) are given by the lengths

$$a = |\mathbf{a}| = \sqrt{\mathbf{a}\cdot\mathbf{a}}, \quad b = |\mathbf{b}| = \sqrt{\mathbf{b}\cdot\mathbf{b}}, \quad c = |\mathbf{c}| = \sqrt{\mathbf{c}\cdot\mathbf{c}}$$

of the basis vectors and by the interaxial angles

$$\alpha = \measuredangle(\mathbf{b}, \mathbf{c}), \quad \beta = \measuredangle(\mathbf{c}, \mathbf{a}), \quad \gamma = \measuredangle(\mathbf{a}, \mathbf{b}).$$

Owing to the relation $\mathbf{v}\cdot\mathbf{w} = |\mathbf{v}|\,|\mathbf{w}|\cos\measuredangle(\mathbf{v}, \mathbf{w})$ for the scalar product of two vectors, one can immediately write down the metric tensor in terms of the cell parameters:

$$\boldsymbol{G} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}.$$

1.3.2.3. Unit cells

A lattice $\mathbf{L}$ can be used to subdivide $\mathbb{V}^3$ into cells of finite volume which all have the same shape. The idea is to define a suitable subset $\mathbf{C}$ of $\mathbb{V}^3$ such that the translates of $\mathbf{C}$ by the vectors in $\mathbf{L}$ cover $\mathbb{V}^3$ without overlapping. Such a subset $\mathbf{C}$ is called a *unit cell* of $\mathbf{L}$, or, in the more mathematically inclined literature, a *fundamental domain* of $\mathbb{V}^3$ with respect to $\mathbf{L}$. Two standard constructions for such unit cells are the *primitive unit cell* and the *Voronoï domain* (which is also known by many other names).

Definition

Let $\mathbf{L}$ be a lattice in $\mathbb{V}^3$ with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

(i) The set $\mathbf{C} := \{x\mathbf{a} + y\mathbf{b} + z\mathbf{c} \mid 0 \le x, y, z < 1\}$ is called the *primitive unit cell* of $\mathbf{L}$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. The primitive unit cell is the parallelepiped spanned by the vectors of the given basis.

(ii) The set $\mathbf{C} := \{\mathbf{w} \in \mathbb{V}^3 \mid |\mathbf{w}| \le |\mathbf{w} - \mathbf{v}| \text{ for all } \mathbf{v} \in \mathbf{L}\}$ is called the *Voronoï domain* or *Dirichlet domain* or *Wigner–Seitz cell* or *Wirkungsbereich* or *first Brillouin zone* (for the case of reciprocal lattices in dual space, see Section 1.3.2.5) of $\mathbf{L}$ (around the origin).

The Voronoï domain consists of those points of $\mathbb{V}^3$ that are closer to the origin than to any other lattice point of $\mathbf{L}$.

See Fig. 1.3.2.2 for examples of these two types of unit cells in two-dimensional space.

It should be noted that the attribute 'primitive' for a unit cell is often omitted. The term 'unit cell' then either denotes a primitive unit cell in the sense of the definition above or a slight generalization of this, namely a cell spanned by vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ which are not necessarily a lattice basis. This will be discussed in detail in the next section. If a unit cell in the even more general sense of a cell whose translates cover the whole space without overlap (thus including *e.g.* Voronoï domains) is meant, this should be indicated by the context.

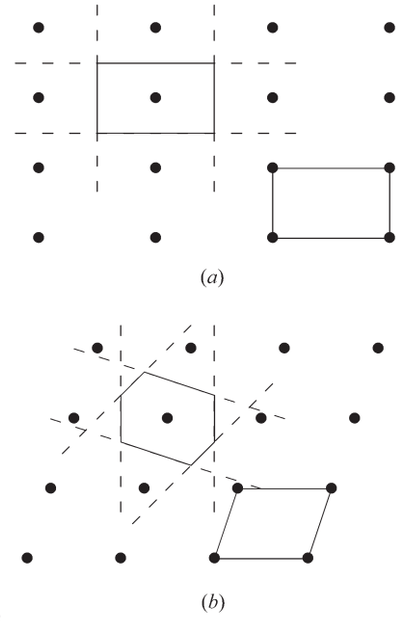

Figure 1.3.2.2
Voronoï domains and primitive unit cells for a rectangular lattice (*a*) and an oblique lattice (*b*).

The construction of the Voronoï domain is independent of the basis of $\mathbf{L}$, as the Voronoï domain is bounded by planes bisecting the line segment between the origin and a lattice point and perpendicular to this segment. In two-dimensional space, the Voronoï domain is simply bounded by lines, in three-dimensional space it is bounded by planes and more generally it is bounded by $(n-1)$-dimensional hyperplanes in n-dimensional space.

The boundaries of the Voronoï domain and its translates overlap, thus in order to get a proper fundamental domain, part of the boundary has to be excluded from the Voronoï domain.

The volume V of the unit cell can be expressed both *via* the metric tensor and *via* the cell parameters. One has

$$\begin{aligned} V^2 &= \det \boldsymbol{G} \\ &= a^2b^2c^2(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma) \end{aligned}$$

and thus

$$V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}.$$

Although the cell parameters depend on the chosen lattice basis, the volume of the unit cell is not affected by a transition to a different lattice basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$. As remarked in Section 1.3.2.1, two lattice bases are related by an integral basis transformation $\boldsymbol{P}$ of determinant ±1 and therefore $\det \boldsymbol{G}' = \det(\boldsymbol{P}^{\mathrm{T}}\cdot\boldsymbol{G}\cdot\boldsymbol{P}) = \det \boldsymbol{G}$, *i.e.* the determinant of the metric tensor is the same for all lattice bases.

Assuming that the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ form a *right-handed* system, the volume can also be obtained *via*

$$V = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a}) = \mathbf{c}\cdot(\mathbf{a}\times\mathbf{b}).$$

1.3.2.4. Primitive and centred lattices

The definition of a lattice as given in Section 1.3.2.1 states that a lattice consists precisely of the integral linear combinations of the vectors in a lattice basis. However, in crystallographic

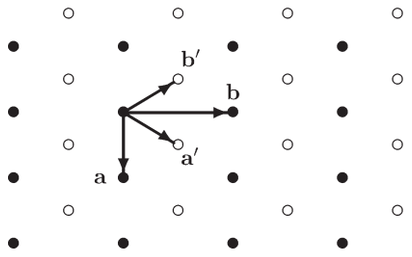

Figure 1.3.2.3
Primitive rectangular lattice (only the filled nodes) and centred rectangular lattice (filled and open nodes).

applications it has turned out to be convenient to work with bases that have particularly nice metric properties. For example, many calculations are simplified if the basis vectors are perpendicular to each other, *i.e.* if the metric tensor has all non-diagonal entries equal to zero. Moreover, it is preferable that the basis vectors reflect the symmetry properties of the lattice. By a case-by-case analysis of the different types of lattices a set of rules for convenient bases has been identified and bases conforming with these rules are called *conventional bases*. The conventional bases are chosen such that in all cases the integral linear combinations of the basis vectors are lattice vectors, but it is admitted that not all lattice vectors are obtained as integral linear combinations.

To emphasize that a basis has the property that the vectors of a lattice are precisely the integral linear combinations of the basis vectors, such a basis is called a *primitive basis* for this lattice.

If the conventional basis of a lattice is not a primitive basis for this lattice, the price to be paid for the transition to the conventional basis is that in addition to the integral linear combinations of the basis vectors one requires one or more *centring vectors* in order to obtain all lattice vectors. These centring vectors have non-integral (but rational) coordinates with respect to the conventional basis. The name *centring* vectors reflects the fact that the additional vectors are usually the centres of the unit cell or of faces of the unit cell spanned by the conventional basis.

Definition

Let $\mathbf{a}, \mathbf{b}, \mathbf{c}$ be linearly independent vectors in $\mathbb{V}^3$.

(i) A lattice $\mathbf{L}$ is called a *primitive lattice* with respect to a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ if $\mathbf{L}$ consists precisely of all integral linear combinations of $\mathbf{a}, \mathbf{b}, \mathbf{c}$, *i.e.* if $\mathbf{L} = \mathbf{L}_P = \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$.

(ii) A lattice $\mathbf{L}$ is called a *centred lattice* with respect to a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ if the integral linear combinations $\mathbf{L}_P = \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$ form a proper sublattice of $\mathbf{L}$ such that $\mathbf{L}$ is the union of $\mathbf{L}_P$ with the translates of $\mathbf{L}_P$ by centring vectors $\mathbf{v}_1, \ldots, \mathbf{v}_s$, *i.e.* $\mathbf{L} = \mathbf{L}_P \cup (\mathbf{v}_1 + \mathbf{L}_P) \cup \ldots \cup (\mathbf{v}_s + \mathbf{L}_P)$.

Typically, the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is a conventional basis and in this case one often briefly says that a lattice $\mathbf{L}$ is a *primitive lattice* or a *centred lattice* without explicitly mentioning the conventional basis.

Example

A rectangular lattice has as conventional basis a vector $\mathbf{a}$ of minimal length and a vector $\mathbf{b}$ of minimal length amongst the vectors perpendicular to $\mathbf{a}$. The resulting primitive lattice $\mathbf{L}_P$ is indicated by the filled nodes in Fig. 1.3.2.3. Now consider the lattice $\mathbf{L}$ having both the filled and the open nodes in Fig. 1.3.2.3 as its lattice nodes. One sees that $\mathbf{a}' = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $\mathbf{b}' = -\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ is a primitive basis for $\mathbf{L}$, but it is more convenient to regard $\mathbf{L}$ as a centred lattice with respect to the basis $\mathbf{a}, \mathbf{b}$ with centring vector $\mathbf{v} = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$. The filled nodes then show the sublattice $\mathbf{L}_P$ of $\mathbf{L}$, the open nodes are the translate $\mathbf{v} + \mathbf{L}_P$ and $\mathbf{L}$ is the union $\mathbf{L}_P \cup (\mathbf{v} + \mathbf{L}_P)$.

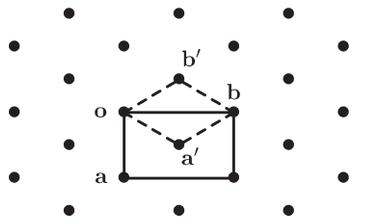

Figure 1.3.2.4
Primitive cell (dashed line) and centred cell (solid lines) for the centred rectangular lattice.

Recalling that a lattice is in particular a group (with addition of vectors as operation), the sublattice $\mathbf{L}_P$ spanned by the basis of a centred lattice is a subgroup of the centred lattice $\mathbf{L}$. Together with the zero vector $\mathbf{v}_0 = \mathbf{0}$, the centring vectors form a set $\mathbf{v}_0, \mathbf{v}_1, \ldots, \mathbf{v}_s$ of coset representatives of $\mathbf{L}$ relative to $\mathbf{L}_P$ and the index $[i]$ of $\mathbf{L}_P$ in $\mathbf{L}$ is $s + 1$. In particular, the sum of two centring vectors is, up to a vector in $\mathbf{L}_P$, again a centring vector, *i.e.* for centring vectors $\mathbf{v}_i$, $\mathbf{v}_j$ there is a unique centring vector $\mathbf{v}_k$ (possibly $\mathbf{0}$) such that $\mathbf{v}_i + \mathbf{v}_j = \mathbf{v}_k + \mathbf{w}$ for a vector $\mathbf{w} \in \mathbf{L}_P$.

The concepts of primitive and centred lattices suggest corresponding notions of primitive and centred unit cells. If $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is a primitive basis for the lattice $\mathbf{L}$, then the parallelepiped spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *primitive unit cell* (or primitive cell); if $\mathbf{a}, \mathbf{b}, \mathbf{c}$ spans a proper sublattice $\mathbf{L}_P$ of index $[i]$ in $\mathbf{L}$, then the parallelepiped spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *centred unit cell* (or centred cell). Since translating a centred cell by translations from the sublattice $\mathbf{L}_P$ covers the full space, the centred cell contains one representative from each coset of the centred lattice $\mathbf{L}$ relative to $\mathbf{L}_P$. This means that the centred cell contains $[i]$ lattice vectors of the centred lattice and due to this a centred cell is also called a *multiple cell*. As a consequence, the volume of the centred cell is $[i]$ times as large as that of a primitive cell for $\mathbf{L}$.

For a conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of the lattice $\mathbf{L}$, the parallelepiped spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a *conventional unit cell* (or conventional cell) of $\mathbf{L}$. Depending on whether the conventional basis is a primitive basis or not, *i.e.* whether the lattice is primitive or centred, the conventional cell is a primitive or a centred cell.

Remark: It is important to note that the cell parameters given in the description of a crystallographic structure almost always refer to a conventional cell. When in the crystallographic literature the term 'unit cell' is used without further attributes, in most cases a conventional unit cell (as specified by the cell parameters) is meant, which is a primitive or centred (multiple) cell depending on whether the lattice is primitive or centred.

Example (continued)

In the example of a centred rectangular lattice, the conventional basis $\mathbf{a}, \mathbf{b}$ spans the centred unit cell indicated by solid lines in Fig. 1.3.2.4, whereas the primitive basis $\mathbf{a}' = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, $\mathbf{b}' = -\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ spans the primitive unit cell indicated by dashed lines. One observes that the centred cell contains two lattice vectors, $\mathbf{o}$ and $\mathbf{a}'$, whereas the primitive cell only contains the zero vector $\mathbf{o}$ (note that due to the condition $0 \leq x, y < 1$ for the points in the unit cell the other vertices

$\mathbf{a}', \mathbf{b}', \mathbf{b}$ of the cell are excluded). The volume of the centred cell is clearly twice as large as that of the primitive cell.

Figures displaying the different primitive and centred unit cells as well as tables describing the metric properties of the different primitive and centred lattices are given in Section 3.1.2.

Examples

(i) The conventional basis for a *primitive cubic lattice* (*cP*) is a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of vectors of equal length which are pairwise perpendicular, *i.e.* with $|\mathbf{a}| = |\mathbf{b}| = |\mathbf{c}|$ and $\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{c} = \mathbf{c} \cdot \mathbf{a} = 0$. As the name indicates, this basis is a primitive basis.

(ii) A *body-centred cubic lattice* (*cI*) has as its conventional basis the conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of a primitive cubic lattice, but the lattice also contains the centring vector $\mathbf{v} = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$ which points to the centre of the conventional cell. If we denote the primitive cubic lattice by $\mathbf{L}_P$, then the body-centred cubic lattice $\mathbf{L}_I$ is the union of $\mathbf{L}_P$ and the translate $\mathbf{v} + \mathbf{L}_P = \{\mathbf{v} + \mathbf{w} \mid \mathbf{w} \in \mathbf{L}_P\}$. Since $\mathbf{L}_P$ is a sublattice of index 2 in $\mathbf{L}_I$, the ratio of the volumes of the centred and the primitive cell of the body-centred cubic lattice is 2.
A possible primitive basis for $\mathbf{L}_I$ is $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$. With respect to this basis, the metric tensor of $\mathbf{L}_I$ is

$$a^2 \cdot \begin{pmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{3}{4} \end{pmatrix}$$

(where $a = \mathbf{a} \cdot \mathbf{a}$). However, it is more common to use a primitive basis with vectors of the same length and equal interaxial angles. Such a basis is $\mathbf{a}'' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}'' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c})$, $\mathbf{c}'' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$ (*cf.* Fig. 1.5.1.3), and with respect to this basis the metric tensor of $\mathbf{L}_I$ is

$$\frac{a^2}{4} \cdot \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

(iii) The conventional basis for a *face-centred cubic lattice* (*cF*) is again the conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of a primitive cubic lattice, but the lattice also contains the three centring vectors $\mathbf{v}_1 = \frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$, $\mathbf{v}_2 = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{c}$, $\mathbf{v}_3 = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ which point to the centres of faces of the conventional cell.
The face-centred cubic lattice $\mathbf{L}_F$ is the union of the primitive cubic lattice $\mathbf{L}_P$ with its translates $\mathbf{v}_i + \mathbf{L}_P$ by the three centring vectors. The ratio of the volumes of the centred and the primitive cell of the face-centred cubic lattice is 4. In this case, the centring vectors actually form a primitive basis of $\mathbf{L}_F$. With respect to the basis $\mathbf{a}' = \frac{1}{2}(\mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b})$ (*cf.* Fig. 1.5.1.4) the metric tensor of $\mathbf{L}_F$ is

$$\frac{a^2}{4} \cdot \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}.$$

(iv) In the conventional basis of a primitive hexagonal lattice, the basis vector $\mathbf{c}$ is chosen as a shortest vector along a sixfold axis. The vectors $\mathbf{a}$ and $\mathbf{b}$ then are shortest vectors along twofold axes in a plane perpendicular to $\mathbf{c}$ and such that they enclose an angle of 120°. The corresponding metric tensor has the form

$$\begin{pmatrix} a^2 & -\frac{a^2}{2} & 0 \\ -\frac{a^2}{2} & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}.$$

(v) In the unit cell of the primitive hexagonal lattice $\mathbf{L}_P$, a point with coordinates $\frac{2}{3}, \frac{1}{3}, z$ is mapped to the points $-\frac{1}{3}, \frac{1}{3}, z$ and $-\frac{1}{3}, -\frac{2}{3}, z$ under the threefold rotation around the c axis. Both of these points are translates of $\frac{2}{3}, \frac{1}{3}, z$ by lattice vectors of $\mathbf{L}_P$. This means that a centring vector of the form $\frac{2}{3}\mathbf{a} + \frac{1}{3}\mathbf{b} + z\mathbf{c}$ will result in a lattice which is invariant under the threefold rotation. Choosing $\mathbf{v}_1 = \frac{1}{3}(2\mathbf{a} + \mathbf{b} + \mathbf{c})$ as centring vector, the lattice generated by $\mathbf{L}_P$ and $\mathbf{v}_1$ contains $\mathbf{L}_P$ as a sublattice of index 3 with coset representatives $\mathbf{0}$, $\mathbf{v}_1$ and $2\mathbf{v}_1 = \frac{1}{3}(4\mathbf{a} + 2\mathbf{b} + 2\mathbf{c})$. The coset representative $2\mathbf{v}_1$ is commonly replaced by $\mathbf{v}_2 = \frac{1}{3}(\mathbf{a} + 2\mathbf{b} + 2\mathbf{c})$ and the centred lattice $\mathbf{L}_R$ with centring vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ so obtained is called the *rhombohedrally centred lattice* (*hR*). The ratio of the volumes of the centred and the primitive cell of the rhombohedrally centred lattice is 3.
For this lattice, the primitive basis of $\mathbf{L}_R$ consisting of three shortest non-coplanar vectors which are permuted by the threefold rotation is also regarded as a conventional basis. With respect to the above lattice basis of the primitive hexagonal lattice, this basis can be chosen as $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$. The metric tensor with respect to this basis is

$$\frac{1}{9} \cdot \begin{pmatrix} 3a^2 + c^2 & -\frac{3}{2}a^2 + c^2 & -\frac{3}{2}a^2 + c^2 \\ -\frac{3}{2}a^2 + c^2 & 3a^2 + c^2 & -\frac{3}{2}a^2 + c^2 \\ -\frac{3}{2}a^2 + c^2 & -\frac{3}{2}a^2 + c^2 & 3a^2 + c^2 \end{pmatrix}.$$

Details about the transformations between hexagonal and rhombohedral lattices are given in Section 1.5.3.1 and Table 1.5.1.1 (see also Fig. 1.5.1.6).

Remark: In three-dimensional space $\mathbb{V}^3$, the conventional bases have been chosen in such a way that any isometry of a centred lattice maps the sublattice generated by the conventional basis to itself. This means that the matrices of the isometries of the lattice are not only integral with respect to a primitive basis, but also when written with respect to the conventional basis. The advantage of the conventional basis is that the matrices are much simpler.

In dimensions $n \geq 4$, such a choice of a conventional basis is in general no longer possible. For example, one will certainly regard the standard orthonormal basis

$$\mathbf{a} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{c} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \mathbf{d} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

of the four-dimensional hypercubic lattice as a conventional basis. The body-centred lattice with centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c} + \mathbf{d})$ is invariant under all the isometries of the hypercubic lattice, but

the body-centred lattice itself allows isometries that do not leave the hypercubic lattice invariant. Thus, not all isometries of the body-centred lattice are integral with respect to the conventional basis of the hypercubic lattice.

1.3.2.5. Reciprocal lattice

For crystallographic applications, a lattice $\mathbf{L}^*$ related to $\mathbf{L}$ is of utmost importance. If the atoms are placed at the nodes of a lattice $\mathbf{L}$, then the diffraction pattern will have sharp Bragg peaks at the nodes of the *reciprocal lattice* $\mathbf{L}^*$. More generally, if the crystal pattern is invariant under translations from $\mathbf{L}$, then the locations of the Bragg peaks in the diffraction pattern will be invariant under translations from $\mathbf{L}^*$.

Definition

Let $\mathbf{L} \subset \mathbb{V}^3$ be a lattice with lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$. Then the *reciprocal basis* $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ is defined by the properties

$$\mathbf{a} \cdot \mathbf{a}^* = \mathbf{b} \cdot \mathbf{b}^* = \mathbf{c} \cdot \mathbf{c}^* = 1$$

and

$$\mathbf{b} \cdot \mathbf{a}^* = \mathbf{c} \cdot \mathbf{a}^* = \mathbf{c} \cdot \mathbf{b}^* = \mathbf{a} \cdot \mathbf{b}^* = \mathbf{a} \cdot \mathbf{c}^* = \mathbf{b} \cdot \mathbf{c}^* = 0,$$

which can conveniently be written as the matrix equation

$$\begin{pmatrix} \mathbf{a} \cdot \mathbf{a}^* & \mathbf{a} \cdot \mathbf{b}^* & \mathbf{a} \cdot \mathbf{c}^* \\ \mathbf{b} \cdot \mathbf{a}^* & \mathbf{b} \cdot \mathbf{b}^* & \mathbf{b} \cdot \mathbf{c}^* \\ \mathbf{c} \cdot \mathbf{a}^* & \mathbf{c} \cdot \mathbf{b}^* & \mathbf{c} \cdot \mathbf{c}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \boldsymbol{I}_3.$$

This means that $\mathbf{a}^*$ is perpendicular to the plane spanned by $\mathbf{b}$ and $\mathbf{c}$ and its projection to the line along $\mathbf{a}$ has length $1/|\mathbf{a}|$. Analogous properties hold for $\mathbf{b}^*$ and $\mathbf{c}^*$.

The *reciprocal lattice* $\mathbf{L}^*$ of $\mathbf{L}$ is defined to be the lattice with lattice basis $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$.

In three-dimensional space $\mathbb{V}^3$, the reciprocal basis can be determined *via* the vector product. Assuming that $\mathbf{a}, \mathbf{b}, \mathbf{c}$ form a right-handed system that spans a unit cell of volume V, the relation $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = V$ and the defining conditions $\mathbf{a} \cdot \mathbf{a}^* = 1$, $\mathbf{b} \cdot \mathbf{a}^* = \mathbf{c} \cdot \mathbf{a}^* = 0$ imply that $\mathbf{a}^* = \frac{1}{V}(\mathbf{b} \times \mathbf{c})$. Analogously, one has $\mathbf{b}^* = \frac{1}{V}(\mathbf{c} \times \mathbf{a})$ and $\mathbf{c}^* = \frac{1}{V}(\mathbf{a} \times \mathbf{b})$.

The reciprocal lattice can also be defined independently of a lattice basis by stating that the vectors of the reciprocal lattice have integral scalar products with all vectors of the lattice:

$$\mathbf{L}^* = \{\mathbf{w}^* \in \mathbb{V}^3 \mid \mathbf{v} \cdot \mathbf{w}^* \in \mathbb{Z} \text{ for all } \mathbf{v} \in \mathbf{L}\}.$$

Owing to the symmetry $\mathbf{v} \cdot \mathbf{w} = \mathbf{w} \cdot \mathbf{v}$ of the scalar product, the roles of the basis and its reciprocal basis can be interchanged. This means that $(\mathbf{L}^*)^* = \mathbf{L}$, *i.e.* taking the reciprocal lattice $(\mathbf{L}^*)^*$ of the reciprocal lattice $\mathbf{L}^*$ results in the original lattice $\mathbf{L}$ again.

Remark: In parts of the literature, especially in physics, the reciprocal lattice is defined slightly differently. The condition there is that $\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi$ if $i = j$ and 0 otherwise and thus the reciprocal lattice is scaled by the factor 2π as compared to the above definition. By this variation the exponential function $\exp(-2\pi i\, \mathbf{v} \cdot \mathbf{w})$ is changed to $\exp(-i\, \mathbf{v} \cdot \mathbf{w})$, which simplifies the formulas for the Fourier transform.

Example

Let $\mathbf{a}, \mathbf{b}, \mathbf{c}$ be the lattice basis of a primitive cubic lattice. Then the body-centred cubic lattice $\mathbf{L}_I$ with centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ is the reciprocal lattice of the rescaled face-centred cubic lattice $2\mathbf{L}_F$, *i.e.* the lattice spanned by $2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$ and the centring vectors $\mathbf{b} + \mathbf{c}$, $\mathbf{a} + \mathbf{c}$, $\mathbf{a} + \mathbf{b}$.

This example illustrates that a lattice and its reciprocal lattice need not have the same type. The reciprocal lattice of a body-centred cubic lattice is a face-centred cubic lattice and *vice versa*. However, the conventional bases are chosen such that for a primitive lattice with a conventional basis as lattice basis, the reciprocal lattice is a primitive lattice of the same type. Therefore the reciprocal lattice of a centred lattice is always a centred lattice for the same type of primitive lattice.

The reciprocal basis can be read off the inverse matrix of the metric tensor $\boldsymbol{G}$: We denote by $\boldsymbol{P}^*$ the matrix containing the coordinate columns of $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$, so that $\mathbf{a}^* = P_{11}^*\mathbf{a} + P_{21}^*\mathbf{b} + P_{31}^*\mathbf{c}$ *etc*. Recalling that scalar products can be computed by multiplying the metric tensor $\boldsymbol{G}$ from the left and right with coordinate columns with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$, the conditions

$$\begin{pmatrix} \mathbf{a} \cdot \mathbf{a}^* & \mathbf{a} \cdot \mathbf{b}^* & \mathbf{a} \cdot \mathbf{c}^* \\ \mathbf{b} \cdot \mathbf{a}^* & \mathbf{b} \cdot \mathbf{b}^* & \mathbf{b} \cdot \mathbf{c}^* \\ \mathbf{c} \cdot \mathbf{a}^* & \mathbf{c} \cdot \mathbf{b}^* & \mathbf{c} \cdot \mathbf{c}^* \end{pmatrix} = \boldsymbol{I}_3$$

defining the reciprocal basis result in the matrix equation $\boldsymbol{I}_3 \cdot \boldsymbol{G} \cdot \boldsymbol{P}^* = \boldsymbol{I}_3$, since the coordinate columns of the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ with respect to itself are the rows of the identity matrix $\boldsymbol{I}_3$, and $\boldsymbol{P}^*$ was just defined to contain the coordinate columns of $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$. But $\boldsymbol{G} \cdot \boldsymbol{P}^* = \boldsymbol{I}_3$ means that $\boldsymbol{P}^* = \boldsymbol{G}^{-1}$ and thus the coordinate columns of $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are precisely the columns of the inverse matrix $\boldsymbol{G}^{-1}$ of the metric tensor $\boldsymbol{G}$.

From $\boldsymbol{P}^* = \boldsymbol{G}^{-1}$ one also derives that the metric tensor $\boldsymbol{G}^*$ of the reciprocal basis is

$$\boldsymbol{G}^* = \boldsymbol{P}^{*\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{P}^* = \boldsymbol{G}^{-1} \cdot \boldsymbol{G} \cdot \boldsymbol{G}^{-1} = \boldsymbol{G}^{-1}.$$

This means that the metric tensors of a basis and its reciprocal basis are inverse matrices of each other. As a further consequence, the volume V^* of the unit cell spanned by the reciprocal basis is $V^* = V^{-1}$, *i.e.* the inverse of the volume of the unit cell spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

Of course, the reciprocal basis can also be computed from the vectors $\mathbf{a}_i$ directly. If $\boldsymbol{B}$ and $\boldsymbol{B}^*$ are the matrices containing as ith column the vectors $\mathbf{a}_i$ and $\mathbf{a}_i^*$, respectively, then the relation defining the reciprocal basis reads as $\boldsymbol{B}^{\mathrm{T}} \cdot \boldsymbol{B}^* = \boldsymbol{I}_3$, *i.e.* $\boldsymbol{B}^* = (\boldsymbol{B}^{-1})^{\mathrm{T}}$. Thus, the reciprocal basis vector $\mathbf{a}_i^*$ is the ith column of the transposed matrix of $\boldsymbol{B}^{-1}$ and thus the ith *row* of the inverse of the matrix $\boldsymbol{B}$ containing the $\mathbf{a}_i$ as columns.

The relations between the parameters of the unit cell spanned by the reciprocal basis vectors and those of the unit cell spanned by the original basis can either be obtained from the vector product expressions for $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ or by explicitly inverting the metric tensor $\boldsymbol{G}$ (*e.g.* using Cramer's rule). The latter approach would also be applicable in n-dimensional space. Either way, one finds

$$a^* = \frac{bc \sin\alpha}{V}, \quad b^* = \frac{ca \sin\beta}{V}, \quad c^* = \frac{ab \sin\gamma}{V},$$
$$\sin\alpha^* = \frac{V}{abc \sin\beta \sin\gamma}, \quad \cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma},$$
$$\sin\beta^* = \frac{V}{abc \sin\gamma \sin\alpha}, \quad \cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha},$$
$$\sin\gamma^* = \frac{V}{abc \sin\alpha \sin\beta}, \quad \cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}.$$

Examples

(i) The lattice **L** spanned by the vectors

$$\mathbf{a} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

has metric tensor

$$\boldsymbol{G} = \begin{pmatrix} 3 & 2 & 0 \\ 2 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

The inverse of the metric tensor is

$$\boldsymbol{G}^* = \boldsymbol{G}^{-1} = \frac{1}{2}\begin{pmatrix} 2 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Interpreting the columns of $\boldsymbol{G}^{-1}$ as coordinate vectors with respect to the original basis, one concludes that the reciprocal basis is given by

$$\mathbf{a}^* = \mathbf{a} - \mathbf{b}, \quad \mathbf{b}^* = \tfrac{1}{2}(-2\mathbf{a} + 3\mathbf{b}), \quad \mathbf{c}^* = \tfrac{1}{2}\mathbf{c}.$$

Inserting the columns for **a**, **b**, **c**, one obtains

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}, \quad \mathbf{c}^* = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

For the direct computation, the matrix $\boldsymbol{B}$ with the basis vectors **a**, **b**, **c** as columns is

$$\boldsymbol{B} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 0 & 0 \end{pmatrix}$$

and has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \frac{1}{2}\begin{pmatrix} 0 & 0 & 2 \\ 1 & 1 & -2 \\ 1 & -1 & 0 \end{pmatrix}.$$

The rows of this matrix are indeed the vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ as computed above.

(ii) The body-centred cubic lattice **L** has the vectors

$$\mathbf{a} = \frac{1}{2}\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \quad \mathbf{c} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}$$

as primitive basis.

The matrix

$$\boldsymbol{B} = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

with the basis vectors **a**, **b**, **c** as columns has as its inverse the matrix

$$\boldsymbol{B}^{-1} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The rows of $\boldsymbol{B}^{-1}$ are the vectors

$$\mathbf{a}^* = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{c}^* = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},$$

showing that the reciprocal lattice of a body-centred cubic lattice is a face-centred cubic lattice.

1.3.3. The structure of space groups

1.3.3.1. Point groups of space groups

The multiplication rule for symmetry operations

$$(\boldsymbol{W}_2,\ \boldsymbol{w}_2)(\boldsymbol{W}_1,\ \boldsymbol{w}_1) = (\boldsymbol{W}_2\boldsymbol{W}_1,\ \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2)$$

shows that the mapping $\Pi : (\boldsymbol{W}, \boldsymbol{w}) \mapsto \boldsymbol{W}$ which assigns a space-group operation to its linear part is actually a group homomorphism, because the first component of the combined operation is simply the product of the linear parts of the two operations. As a consequence, the linear parts of a space group form a group themselves, which is called the point group of $\mathcal{G}$. The kernel of the homomorphism Π consists precisely of the translations $(\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}$, and since kernels of homomorphisms are always normal subgroups (*cf.* Section 1.1.6), the translation subgroup $\mathcal{T}$ forms a normal subgroup of $\mathcal{G}$. According to the *homomorphism theorem* (see Section 1.1.6), the point group is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$.

Definition

The *point group* $\mathcal{P}$ of a space group $\mathcal{G}$ is the group of linear parts of operations occurring in $\mathcal{G}$. It is isomorphic to the factor group $\mathcal{G}/\mathcal{T}$ of $\mathcal{G}$ by the translation subgroup $\mathcal{T}$.

When $\mathcal{G}$ is considered with respect to a coordinate system, the operations of $\mathcal{P}$ are simply 3×3 matrices.

The point group plays an important role in the analysis of the macroscopic properties of crystals: it describes the symmetry of the set of face normals and can thus be directly observed. It is usually obtained from the *diffraction record* of the crystal, where adding the information about the translation subgroup explains the sharpness of the Bragg peaks in the diffraction pattern.

Although we have already deduced that the translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ forms a normal subgroup in $\mathcal{G}$ because it is the kernel of the homomorphism mapping each operation to its linear part, it is worth investigating this fact by an explicit computation. Let $t = (\boldsymbol{I},\ \boldsymbol{t})$ be a translation in $\mathcal{T}$ and $W = (\boldsymbol{W},\ \boldsymbol{w})$ an arbitrary operation in $\mathcal{G}$, then one has

$$\begin{aligned} WtW^{-1} &= (\boldsymbol{W},\ \boldsymbol{w})(\boldsymbol{I},\ \boldsymbol{t})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{W},\ \boldsymbol{W}\boldsymbol{t} + \boldsymbol{w})(\boldsymbol{W}^{-1},\ -\boldsymbol{W}^{-1}\boldsymbol{w}) \\ &= (\boldsymbol{I},\ -\boldsymbol{w} + \boldsymbol{W}\boldsymbol{t} + \boldsymbol{w}) = (\boldsymbol{I},\ \boldsymbol{W}\boldsymbol{t}), \end{aligned}$$

which is again a translation in $\mathcal{G}$, namely by $\boldsymbol{W}\boldsymbol{t}$. This little computation shows an important property of the translation subgroup with respect to the point group, namely that every vector from the translation lattice is mapped again to a lattice vector by each operation of the point group of $\mathcal{G}$.

Proposition. Let $\mathcal{G}$ be a space group with point group $\mathcal{P}$ and translation subgroup $\mathcal{T}$ and let $\mathbf{L} = \{\boldsymbol{t} \mid (\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}\}$ be the lattice of translations in $\mathcal{T}$. Then $\mathcal{P}$ acts on the lattice **L**, *i.e.* for every $\boldsymbol{W} \in \mathcal{P}$ and $\boldsymbol{t} \in \mathbf{L}$ one has $\boldsymbol{W}\boldsymbol{t} \in \mathbf{L}$.

A point group that acts on a lattice is a subgroup of the full group of symmetries of the lattice, obtained as the group of orthogonal mappings that map the lattice to itself. With respect to a primitive basis, the group of symmetries of a lattice consists of all integral basis transformations that fix the metric tensor of the lattice.

Definition

Let **L** be a three-dimensional lattice with metric tensor $\boldsymbol{G}$ with respect to a primitive basis **a**, **b**, **c**.

(i) An *automorphism* of **L** is an isometry mapping **L** to itself. Written with respect to the basis **a**, **b**, **c**, an automorphism of **L** is an integral basis transformation fixing the metric tensor of **L**, *i.e.* it is an integral matrix $\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z})$ with $\boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$.

(ii) The group

$$\mathcal{B} := Aut(\mathbf{L}) = \{\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z}) \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}\}$$

of all automorphisms of **L** is called the *automorphism group* or *Bravais group* of **L**. Note that $Aut(\mathbf{L})$ acts on the coordinate columns of **L**, which are simply columns with integral coordinates.

Since the isometries in the Bravais group of a lattice preserve distances, the possible images of the vectors in a basis are vectors of the same lengths as the basis vectors. But due to its discreteness, a lattice contains only finitely many lattice vectors up to a given length. This means that a lattice automorphism can only permute the finitely many vectors up to the maximum length of a basis vector. Thus, there can only be finitely many automorphisms of a lattice. This argument proves the following important fact:

Theorem. The Bravais group of a lattice is finite. As a consequence, point groups of space groups are finite groups.

As subgroups of the Bravais group of a lattice, point groups can be realized as integral matrix groups when written with respect to a primitive basis. For a centred lattice, it is possible that the Bravais group of a lattice contains non-integral matrices, because the centring vector is a column with non-integral entries. However, in dimensions two and three the conventional bases are chosen such that the Bravais groups of all lattices are integral when written with respect to a conventional basis.

Information on the Bravais groups of the primitive lattices in two- and three-dimensional space is displayed in Tables 1.3.3.1 and 1.3.3.2. The columns of the tables contain the names of the lattices, the metric tensor with respect to the conventional basis (with only the upper half given, the lower half following by the symmetry of the metric tensor), the Hermann–Mauguin symbol for the type of the Bravais group and generators of the Bravais group (given in the shorthand notation introduced in Section 1.2.2.1 and the corresponding Seitz symbols discussed in Section 1.4.2.2).

The finiteness and integrality of the point groups has important consequences. For example, it implies the *crystallographic restriction* that rotations in space groups of two- and three-dimensional space can only have orders 1, 2, 3, 4 or 6. On the one hand, an integral matrix clearly has an integral trace.[1] But a matrix $\boldsymbol{W}$ with the property that $\boldsymbol{W}^k = \boldsymbol{I}$ can be diagonalized over the complex numbers and the diagonal entries have to be kth roots of unity, *i.e.* powers of $\zeta_k = \exp(2\pi i/k)$. Since diagonalization does not change the trace, the sum of these kth roots of unity still has to be an integer and in particular these roots of unity have to occur in complex conjugate pairs. In dimension 2 this means that the two diagonal entries are complex conjugate and the only possible ways to obtain an integral trace are $\zeta_1 + \zeta_1^{-1} = 2$, $\zeta_2 + \zeta_2^{-1} = -2$, $\zeta_3 + \zeta_3^{-1} = -1$, $\zeta_4 + \zeta_4^{-1} = 0$ and $\zeta_6 + \zeta_6^{-1} = 1$. In dimension 3 the third diagonal entry does not have a complex conjugate partner, and therefore has to be ± 1.

[1] The trace of a matrix is the sum of its diagonal entries.

Table 1.3.3.1
Automorphism groups of two-dimensional primitive lattices

Lattice	Metric tensor	Bravais group: Hermann–Mauguin symbol	Bravais group: Generators
Oblique	$\begin{pmatrix} g_{11} & g_{12} \\ & g_{22} \end{pmatrix}$	2	2: $\bar{x}, \bar{y}$
Rectangular	$\begin{pmatrix} g_{11} & 0 \\ & g_{22} \end{pmatrix}$	2*mm*	2: $\bar{x}, \bar{y}$ m_{10}: $\bar{x}, y$
Square	$\begin{pmatrix} g_{11} & 0 \\ & g_{11} \end{pmatrix}$	4*mm*	4^+: $\bar{y}, x$ m_{10}: $\bar{x}, y$
Hexagonal	$\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} \\ & g_{11} \end{pmatrix}$	6*mm*	6^+: $x - y, x$ m_{21}: $\bar{x}, \bar{x} + y$

Thus the possible orders in dimension 3 are the same as in dimension 2.

A much stronger result was obtained by H. Minkowski (1887). He gave an explicit bound for the maximal power p^m of a prime p which can divide the order of an n-dimensional finite integral matrix group. In dimension 2 this theorem implies that the orders of the point groups divide 24 and in dimension 3 the orders of the point groups divide 48. The Bravais groups 4*mm* (of order 8) and 6*mm* (of order 12) of the square and hexagonal lattices in dimension 2 and the Bravais group $m\bar{3}m$ (of order 48) of the cubic lattice in dimension 3 show that Minkowski's result is the best possible in these dimensions.

1.3.3.2. Coset decomposition with respect to the translation subgroup

The translation subgroup $\mathcal{T}$ of a space group $\mathcal{G}$ can be used to distribute the operations of $\mathcal{G}$ into different classes by grouping together all operations that differ only by a translation. This results in the decomposition of $\mathcal{G}$ into cosets with respect to $\mathcal{T}$ (see Section 1.1.4 for details of cosets).

Definition

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$.

(i) The *right coset* $\mathcal{T}W$ of an operation $W \in \mathcal{G}$ with respect to $\mathcal{T}$ is the set $\{tW \mid t \in \mathcal{T}\}$.
Analogously, the set $W\mathcal{T} = \{Wt \mid t \in \mathcal{T}\}$ is called the *left coset* of W with respect to $\mathcal{T}$.

(ii) A set $\{W_1, \ldots, W_m\}$ of operations in $\mathcal{G}$ is called a system of *coset representatives* relative to $\mathcal{T}$ if every operation W in $\mathcal{G}$ is contained in exactly one coset $\mathcal{T}W_i$.

(iii) Writing $\mathcal{G}$ as the disjoint union

$$\mathcal{G} = \mathcal{T}W_1 \cup \ldots \cup \mathcal{T}W_m$$

is called the *coset decomposition of* $\mathcal{G}$ *relative to* $\mathcal{T}$.

If the translation subgroup $\mathcal{T}$ is a subgroup of index $[i]$ in $\mathcal{G}$, a set of coset representatives for $\mathcal{G}$ relative to $\mathcal{T}$ consists of $[i]$ operations $W_1, W_2, \ldots, W_{[i]}$, where W_1 is assumed to be the identity element e of $\mathcal{G}$. The cosets of $\mathcal{G}$ relative to $\mathcal{T}$ can be imagined as columns of an infinite array with $[i]$ columns, labelled by the coset representatives, as displayed in Table 1.3.3.3.

Table 1.3.3.2
Automorphism groups of three-dimensional primitive lattices

Lattice	Metric tensor	Bravais group	
		Hermann–Mauguin symbol	Generators
Triclinic	$\begin{pmatrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{pmatrix}$	$\bar{1}$	$\bar{1}$: $\bar{x}, \bar{y}, \bar{z}$
Monoclinic	$\begin{pmatrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$	$2/m$	2_{010}: $\bar{x}, y, \bar{z}$ m_{010}: $x, \bar{y}, z$
Orthorhombic	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$	mmm	m_{100}: $\bar{x}, y, z$ m_{010}: $x, \bar{y}, z$ m_{001}: $x, y, \bar{z}$
Tetragonal	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{pmatrix}$	$4/mmm$	4_{001}: $\bar{y}, x, z$ m_{001}: $x, y, \bar{z}$ m_{100}: $\bar{x}, y, z$
Hexagonal	$\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{pmatrix}$	$6/mmm$	6_{001}: $x-y, x, z$ m_{001}: $x, y, \bar{z}$ m_{100}: $\bar{x}+y, y, z$
Rhombohedral	$\begin{pmatrix} g_{11} & g_{12} & g_{12} \\ & g_{11} & g_{12} \\ & & g_{11} \end{pmatrix}$	$\bar{3}m$	$\bar{3}_{111}$: $\bar{z}, \bar{x}, \bar{y}$ $m_{1\bar{1}0}$: y, x, z
Cubic	$\begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{pmatrix}$	$m\bar{3}m$	m_{001}: $x, y, \bar{z}$ $\bar{3}_{111}$: $\bar{z}, \bar{x}, \bar{y}$ m_{110}: $\bar{y}, \bar{x}, z$

Table 1.3.3.3
Right-coset decomposition of $\mathcal{G}$ relative to $\mathcal{T}$

$W_1 = e$	W_2	W_3	...	$W_{[i]}$
t_1	$t_1 W_2$	$t_1 W_3$	...	$t_1 W_{[i]}$
t_2	$t_2 W_2$	$t_2 W_3$	...	$t_2 W_{[i]}$
t_3	$t_3 W_2$	$t_3 W_3$	...	$t_3 W_{[i]}$
t_4	$t_4 W_2$	$t_4 W_3$	...	$t_4 W_{[i]}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$

Remark: We can assume some enumeration $t_1, t_2, t_3, \ldots$ of the operations in $\mathcal{T}$ because the translation vectors form a lattice. For example, with respect to a primitive basis, the coordinate vectors of the translations in $\mathcal{G}$ are simply columns $\begin{pmatrix} l \\ m \\ n \end{pmatrix}$ with integral components l, m, n. A straightforward enumeration of these columns would start with

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} \bar{1} \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \bar{1} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \bar{1} \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \ldots$$

Writing out the matrix–column pairs, the coset $\mathcal{T}(\boldsymbol{W}, \boldsymbol{w})$ consists of the operations of the form $(\boldsymbol{I}, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t})$ with $\boldsymbol{t}$ running over the lattice translations of $\mathcal{T}$. This means that the operations of a coset with respect to the translation subgroup all have the same linear part, which is also evident from a listing of the cosets as columns of an infinite array, as in the example above.

Proposition

Let $W = (\boldsymbol{W}, \boldsymbol{w})$ and $W' = (\boldsymbol{W}', \boldsymbol{w}')$ be two operations of a space group $\mathcal{G}$ with translation subgroup $\mathcal{T}$.

(1) If $\boldsymbol{W} \neq \boldsymbol{W}'$, then the cosets $\mathcal{T}W$ and $\mathcal{T}W'$ are disjoint, *i.e.* their intersection is empty.

(2) If $\boldsymbol{W} = \boldsymbol{W}'$, then the cosets $\mathcal{T}W$ and $\mathcal{T}W'$ are equal, because WW'^{-1} has linear part $\boldsymbol{I}$ and is thus an operation contained in $\mathcal{T}$.

The one-to-one correspondence between the point-group operations and the cosets relative to $\mathcal{T}$ explicitly displays the isomorphism between the point group $\mathcal{P}$ of $\mathcal{G}$ and the factor group $\mathcal{G}/\mathcal{T}$. This correspondence is also exploited in the listing of the general-position coordinates. What is given there are the coordinate triplets for coset representatives of $\mathcal{G}$ relative to $\mathcal{T}$, which correspond to the first row of the array in Table 1.3.3.3. As just explained, the other operations in $\mathcal{G}$ can be obtained from these coset representatives by adding a lattice translation to the translational part.

Furthermore, the correspondence between the point group and the coset decomposition relative to $\mathcal{T}$ makes it easy to find a system of coset representatives $\{W_1, \ldots, W_m\}$ of $\mathcal{G}$ relative to $\mathcal{T}$. What is required is that the linear parts of the W_i are precisely the operations in the point group of $\mathcal{G}$. If $\boldsymbol{W}_1, \ldots, \boldsymbol{W}_m$ are the different operations in the point group $\mathcal{P}$ of $\mathcal{G}$, then a system of coset representatives is obtained by choosing for every linear part $\boldsymbol{W}_i$ a translation part $\boldsymbol{w}_i$ such that $W_i = (\boldsymbol{W}_i, \boldsymbol{w}_i)$ is an operation in $\mathcal{G}$.

It is customary to choose the translation parts $\boldsymbol{w}_i$ of the coset representatives such that their coordinates lie between 0 and 1,

excluding 1. In particular, if the translation part of a coset representative is a lattice vector, it is usually chosen as the zero vector $\boldsymbol{o}$.

Note that due to the fact that $\mathcal{T}$ is a normal subgroup of $\mathcal{G}$, a system of coset representatives for the right cosets is at the same time a system of coset representatives for the left cosets.

1.3.3.3. Symmorphic and non-symmorphic space groups

If a coset with respect to the translation subgroup contains an operation of the form $(\boldsymbol{W}, \boldsymbol{w})$ with $\boldsymbol{w}$ a vector in the translation lattice, it is clear that the same coset also contains the operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part. On the other hand, if a coset does not contain an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$, this may be caused by an inappropriate choice of origin. For example, the operation $(-\boldsymbol{I}, (1/2, 1/2, 1/2))$ is turned into the inversion $(-\boldsymbol{I}, (0, 0, 0))$ by moving the origin to $1/4, 1/4, 1/4$ (*cf.* Section 1.5.1.1 for a detailed treatment of origin-shift transformations).

Depending on the actual space group $\mathcal{G}$, it may or may not be possible to choose the origin such that every coset with respect to $\mathcal{T}$ contains an operation of the form $(\boldsymbol{W}, \boldsymbol{o})$.

Definition

Let $\mathcal{G}$ be a space group with translation subgroup $\mathcal{T}$. If it is possible to choose the coordinate system such that every coset of $\mathcal{G}$ with respect to $\mathcal{T}$ contains an operation $(\boldsymbol{W}, \boldsymbol{o})$ with trivial translation part, $\mathcal{G}$ is called a *symmorphic* space group, otherwise $\mathcal{G}$ is called a *non-symmorphic* space group.

One sees that the operations with trivial translation part form a subgroup of $\mathcal{G}$ which is isomorphic to a subgroup of the point group $\mathcal{P}$. This subgroup is the group of operations in $\mathcal{G}$ that fix the origin and is called the *site-symmetry group* of the origin (site-symmetry groups are discussed in detail in Section 1.4.4). It is the distinctive property of symmorphic space groups that they contain a subgroup which is isomorphic to the full point group. This may in fact be seen as an alternative definition for symmorphic space groups.

Proposition. A space group $\mathcal{G}$ with point group $\mathcal{P}$ is symmorphic if and only if it contains a subgroup isomorphic to $\mathcal{P}$. For a non-symmorphic space group $\mathcal{G}$, every finite subgroup of $\mathcal{G}$ is isomorphic to a proper subgroup of the point group.

Note that every finite subgroup of a space group is a subgroup of the site-symmetry group for some point, because finite groups cannot contain translations. Therefore, a symmorphic space group is characterized by the fact that it contains a site-symmetry group isomorphic to its point group, whereas in non-symmorphic space groups all site-symmetry groups have orders strictly smaller than the order of the point group.

Symmorphic space groups can easily be constructed by choosing a lattice $\mathbf{L}$ and a point group $\mathcal{P}$ which acts on $\mathbf{L}$. Then $\mathcal{G} = \{(\boldsymbol{W}, \boldsymbol{w}) \mid \boldsymbol{W} \in \mathcal{P}, \boldsymbol{w} \in \mathbf{L}\}$ is a space group in which the coset representatives can be chosen as $(\boldsymbol{W}, \boldsymbol{o})$.

Non-symmorphic space groups can also be constructed from a lattice $\mathbf{L}$ and a point group $\mathcal{P}$. What is required is a system of coset representatives with respect to $\mathcal{T}$ and these are obtained by choosing for each operation $\boldsymbol{W} \in \mathcal{P}$ a translation part $\boldsymbol{w}$. Owing to the translations, it is sufficient to consider vectors $\boldsymbol{w}$ with components between 0 and 1. However, the translation parts cannot be chosen arbitrarily, because for a point-group operation of order k, the operation $(\boldsymbol{W}, \boldsymbol{w})^k$ has to be a translation $(\boldsymbol{I}, \boldsymbol{t})$ with $\boldsymbol{t} \in \mathbf{L}$. Working this out, this imposes the restriction that

$$(\boldsymbol{W}^{k-1} + \ldots + \boldsymbol{W} + \boldsymbol{I})\boldsymbol{w} \in \mathbf{L}.$$

Once translation parts $\boldsymbol{w}$ are found that fulfil all these restrictions, one finally has to check whether the space group obtained this way is (by accident) symmorphic, but written with respect to an inappropriate origin. A change of origin by $\boldsymbol{p}$ is realized by conjugating the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ by the translation $(\boldsymbol{I}, -\boldsymbol{p})$ (*cf.* Section 1.5.1 on transformations of the coordinate system) which gives

$$(\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}, \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{W}\boldsymbol{p} + \boldsymbol{w} - \boldsymbol{p}) = (\boldsymbol{W}, \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}).$$

Thus, the space group just constructed is symmorphic if there is a vector $\boldsymbol{p}$ such that $(\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p} + \boldsymbol{w} \in \mathbf{L}$ for each of the coset representatives $(\boldsymbol{W}, \boldsymbol{w})$.

The above considerations also show how every space group can be assigned to a symmorphic space group in a canonical way, namely by setting the translation parts of coset representatives with respect to $\mathcal{T}$ to $\boldsymbol{o}$. This has the effect that screw rotations are turned into rotations and glide reflections into reflections. The Hermann–Mauguin symbol (see Section 1.4.1 for a detailed discussion of Hermann–Mauguin symbols) of the symmorphic space group to which an arbitrary space group is assigned is simply obtained by replacing any screw rotation symbol N_m by the corresponding rotation symbol N and every glide reflection symbol a, b, c, d, e, n by the symbol m for a reflection. A space group is found to be symmorphic if no such replacement is required, *i.e.* if the Hermann–Mauguin symbol only contains the symbols 1, 2, 3, 4, 6 for rotations, $\bar{1}$, $\bar{3}$, $\bar{4}$, $\bar{6}$ for rotoinversions and m for reflections.

Example

The space groups with Hermann-Mauguin symbols $P4mm$, $P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$, $P4_2bc$ are all assigned to the symmorphic space group with Hermann–Mauguin symbol $P4mm$.

1.3.4. Classification of space groups

In this section we will consider various ways in which space groups may be grouped together. For the space groups themselves, the natural notion of equivalence is the classification into *space-group types*, but the point groups and lattices from which the space groups are built also have their own classification schemes into *geometric crystal classes* and *Bravais types of lattices*, respectively.

Some other types of classifications are relevant for certain applications, and these will also be considered. The hierarchy of the different classification levels and the numbers of classes on the different levels in dimension 3 are displayed in Fig. 1.3.4.1.

1.3.4.1. Space-group types

The main motivation behind studying space groups is that they allow the classification of crystal structures according to their symmetry properties. Since many properties of a structure can be derived from its group of symmetries alone, this allows the investigation of the properties of many structures simultaneously.

On the other hand, even for the same crystal structure the corresponding space group may look different, depending on the chosen coordinate system (see Chapter 1.5 for a detailed discussion of transformations to different coordinate systems). Because it is natural to regard two realizations of a group of symmetry operations with respect to two different coordinate systems as equivalent, the following notion of equivalence between space groups is natural.

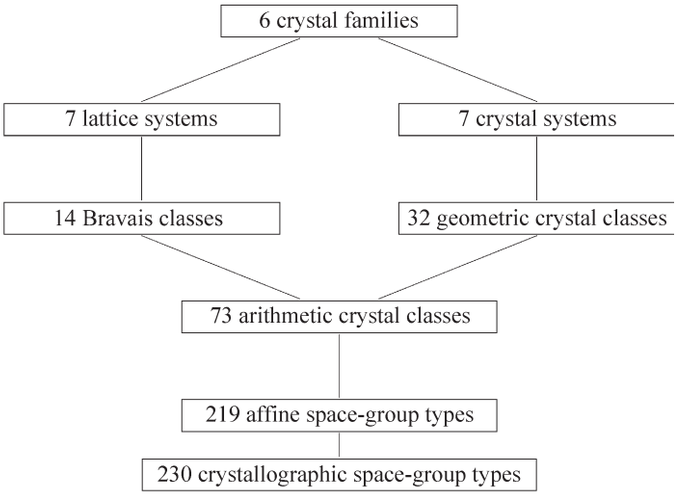

Figure 1.3.4.1
Classification levels for three-dimensional space groups.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are called *affinely equivalent* if $\mathcal{G}'$ can be obtained from $\mathcal{G}$ by a change of the coordinate system. In terms of matrix–column pairs this means that there must exist a matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ such that

$$\mathcal{G}' = \{(\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p}) \mid (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}\}.$$

The collection of space groups that are affinely equivalent with $\mathcal{G}$ forms the *affine type* of $\mathcal{G}$.

In dimension 2 there are 17 affine types of plane groups and in dimension 3 there are 219 affine space-group types. Note that in order to avoid misunderstandings we refrain from calling the space-group types *affine classes*, since the term classes is usually associated with *geometric crystal classes* (see below).

Grouping together space groups according to their space-group type serves different purposes. On the one hand, it is sometimes convenient to consider the same crystal structure and thus also its space group with respect to different coordinate systems, *e.g.* when the origin can be chosen in different natural ways or when a phase transition to a higher- or lower-symmetry phase with a different conventional cell is described. On the other hand, different crystal structures may give rise to the same space group once suitable coordinate systems have been chosen for both. We illustrate both of these perspectives by an example.

Examples

(i) The space group $\mathcal{G}$ of type *Pban* (50) has a subgroup $\mathcal{H}$ of index 2 for which the coset representatives relative to the translation subgroup are the identity e: x, y, z, the twofold rotation g: $-x, y, -z$, the n glide h: $x+\frac{1}{2}, y+\frac{1}{2}, -z$ and the b glide k: $-x+\frac{1}{2}, y+\frac{1}{2}, z$. This subgroup is of type *Pb*2*n*, which is a non-conventional setting for *Pnc*2 (30). In the conventional setting, the coset representatives of *Pnc*2 are given by g': $-x, -y, z$, h': $-x, y+\frac{1}{2}, z+\frac{1}{2}$ and k': $x, -y+\frac{1}{2}, z+\frac{1}{2}$, *i.e.* with the z axis as rotation axis for the twofold rotation. The subgroup $\mathcal{H}$ can be transformed to its conventional setting by the basis transformation $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{c}, \mathbf{a}, \mathbf{b})$. Depending on whether the perspective of the full group $\mathcal{G}$ or the subgroup $\mathcal{H}$ is more important for a crystal structure, the groups $\mathcal{G}$ and $\mathcal{H}$ will be considered either with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ (conventional for $\mathcal{G}$) or to the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ (conventional for $\mathcal{H}$).

(ii) The elements carbon, silicon and germanium all crystallize in the *diamond structure*, which has a face-centred cubic unit cell with two atoms shifted by 1/4 along the space diagonal of the conventional cubic cell. The space group is in all cases of type $Fd\bar{3}m$ (227), but the cell parameters differ: $a_{\rm C} = 3.5668$ Å for carbon, $a_{\rm Si} = 5.4310$ Å for silicon and $a_{\rm Ge} = 5.6579$ Å for germanium (measured at 298 K). In order to scale the conventional cell of carbon to that of silicon, the coordinate system has to be transformed by the diagonal matrix

$$a_{\rm Si}/a_{\rm C} \cdot \boldsymbol{I}_3 \approx \begin{pmatrix} 1.523 & 0 & 0 \\ 0 & 1.523 & 0 \\ 0 & 0 & 1.523 \end{pmatrix}.$$

By a famous theorem of Bieberbach (see Bieberbach, 1911, 1912), affine equivalence of space groups actually coincides with the notion of abstract group isomorphism as discussed in Section 1.1.6.

Bieberbach theorem

Two space groups in n-dimensional space are isomorphic if and only if they are conjugate by an affine mapping.

This theorem is by no means obvious. Recall that for point groups the situation is very different, since for example the abstract cyclic group of order 2 is realized in the point groups of space groups of type $P2$, Pm and $P\bar{1}$, generated by a twofold rotation, reflection and inversion, respectively, which are clearly not equivalent in any geometric sense. The driving force behind the Bieberbach theorem is the special structure of space groups having an infinite normal translation subgroup on which the point group acts.

In crystallography, a notion of equivalence slightly stronger than affine equivalence is usually used. Since crystals occur in physical space and physical space can only be transformed by orientation-preserving mappings, space groups are only regarded as equivalent if they are conjugate by an *orientation-preserving* coordinate transformation, *i.e.* by an affine mapping that has a linear part with positive determinant.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are said to belong to the same *space-group type* if $\mathcal{G}'$ can be obtained from $\mathcal{G}$ by an orientation-preserving coordinate transformation, *i.e.* by conjugation with a matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ with $\det \boldsymbol{P} > 0$. In order to distinguish the space-group types explicitly from the affine space-group types (corresponding to the isomorphism classes), they are often called *crystallographic space-group types*.

The (crystallographic) space-group type collects together the infinitely many space groups that are obtained by expressing a single space group with respect to all possible right-handed coordinate systems for the point space.

Example

We consider the space group $\mathcal{G}$ of type $I4_1$ (80) which is generated by the right-handed fourfold screw rotation g: $-y, x+1/2, z+1/4$ (located at $-1/4, 1/4, z$), the centring translation t: $x+1/2, y+1/2, z+1/2$ and the integral translations of a primitive tetragonal lattice. Conjugating the group $\mathcal{G}$ to $\mathcal{G}' = m\mathcal{G}m^{-1}$ by the reflection m in the plane $z = 0$ turns the right-handed screw rotation g into the left-handed screw

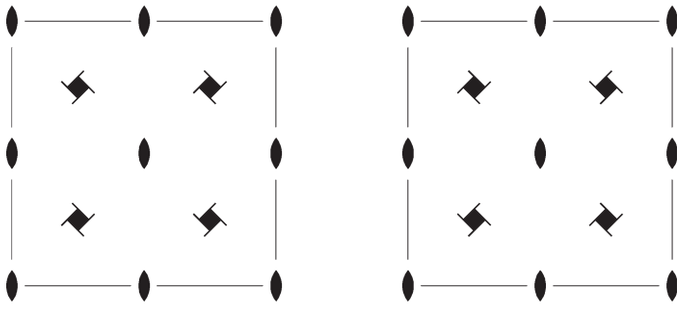

Figure 1.3.4.2
Space-group diagram of $I4_1$ (left) and its reflection in the plane $z = 0$ (right).

rotation g': $-y, x + 1/2, z - 1/4$, and one might suspect that $\mathcal{G}'$ is a space group of the same affine type but of a different crystallographic space-group type as $\mathcal{G}$. However, this is not the case because conjugating $\mathcal{G}$ by the translation $n = t(0, 1/2, 0)$ conjugates g to $g'' = ngn^{-1}$: $-y + 1/2$, $x + 1, z + 1/4$. One sees that g'' is the composition of g' with the centring translation t and hence g'' belongs to $\mathcal{G}'$. This shows that conjugating $\mathcal{G}$ by either the reflection m or the translation n both result in the same group $\mathcal{G}'$. This can also be concluded directly from the space-group diagrams in Fig. 1.3.4.2. Reflecting in the plane $z = 0$ turns the diagram on the left into the diagram on the right, but the same effect is obtained when the left diagram is shifted by $\frac{1}{2}$ along either **a** or **b**.

The groups $\mathcal{G}$ and $\mathcal{G}'$ thus belong to the same crystallographic space-group type because $\mathcal{G}$ is transformed to $\mathcal{G}'$ by a shift of the origin by $\frac{1}{2}$**b**, which is clearly an orientation-preserving coordinate transformation.

Enantiomorphism

The 219 affine space-group types in dimension 3 result in 230 crystallographic space-group types. Since an affine type either forms a single space-group type (in the case where the group obtained by an orientation-reversing coordinate transformation can also be obtained by an orientation-preserving transformation) or splits into two space-group types, this means that there are 11 affine space-group types such that an orientation-reversing coordinate transformation cannot be compensated by an orientation-preserving transformation.

Groups that differ only by their handedness are closely related to each other and share many properties. One addresses this phenomenon by the concept of *enantiomorphism*.

Example

Let $\mathcal{G}$ be a space group of type $P4_1$ (76) generated by a fourfold right-handed screw rotation $(4^+_{001}, (0, 0, 1/4))$ and the translations of a primitive tetragonal lattice. Then transforming the coordinate system by a reflection in the plane $z = 0$ results in a space group $\mathcal{G}'$ with fourfold left-handed screw rotation $(4^-_{001}, (0, 0, 1/4)) = (4^+_{001}, (0, 0, -1/4))^{-1}$. The groups $\mathcal{G}$ and $\mathcal{G}'$ are isomorphic because they are conjugate by an affine mapping, but $\mathcal{G}'$ belongs to a different space-group type, namely $P4_3$ (78), because $\mathcal{G}$ does not contain a fourfold left-handed screw rotation with translation part $\frac{1}{4}$**c**.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ are said to form an *enantiomorphic pair* if they are conjugate under an affine mapping, but not under an orientation-preserving affine mapping.

If $\mathcal{G}$ is the group of isometries of some crystal pattern, then its enantiomorphic counterpart $\mathcal{G}'$ is the group of isometries of the mirror image of this crystal pattern.

The splitting of affine space-group types of three-dimensional space groups into pairs of crystallographic space-group types gives rise to the following 11 enantiomorphic pairs of space-group types: $P4_1/P4_3$ (76/78), $P4_122/P4_322$ (91/95), $P4_12_12/P4_32_12$ (92/96), $P3_1/P3_2$ (144/145), $P3_112/P3_212$ (151/153), $P3_121/P3_221$ (152/154), $P6_1/P6_5$ (169/173), $P6_2/P6_4$ (170/172), $P6_122/P6_522$ (178/179), $P6_222/P6_422$ (180/181), $P4_332/P4_132$ (212/213). These groups are easily recognized by their Hermann–Mauguin symbols, because they are the primitive groups for which the Hermann–Mauguin symbol contains one of the screw rotations 3_1, 3_2, 4_1, 4_3, 6_1, 6_2, 6_4 or 6_5. The groups with fourfold screw rotations and body-centred lattices do not give rise to enantiomorphic pairs, because in these groups the orientation reversal can be compensated by an origin shift, as illustrated in the example above for the group of type $I4_1$.

Example

A well known example of a crystal that occurs in forms whose symmetry is described by enantiomorphic pairs of space groups is quartz. For low-temperature α-quartz there exists a left-handed and a right-handed form with space groups $P3_121$ (152) and $P3_221$ (154), respectively. The two individuals of opposite chirality occur together in the so-called Brazil twin of quartz. At higher temperatures, a phase transition leads to the higher-symmetry β-quartz forms, with space groups $P6_422$ (181) and $P6_222$ (180), which still form an enantiomorphic pair.

1.3.4.2. Geometric crystal classes

We recall that the point group of a space group is the group of linear parts occurring in the space group. Once a basis for the underlying vector space is chosen, such a point group is a group of 3×3 matrices. A point group is characterized by the relative positions between the rotation and rotoinversion axes and the reflection planes of the operations it contains, and in this sense a point group is independent of the chosen basis. However, a suitable choice of basis is useful to highlight the geometric properties of a point group.

Example

A point group of type $3m$ is generated by a threefold rotation and a reflection in a plane with normal vector perpendicular to the rotation axis. Choosing a basis **a**, **b**, **c** such that **c** is along the rotation axis, **a** is perpendicular to the reflection plane and **b** is the image of **a** under the threefold rotation (*i.e.* **b** lies in the plane perpendicular to the rotation axis and makes an angle of 120° with **a**), the matrices of the threefold rotation and the reflection with respect to this basis are

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

A different useful basis is obtained by choosing a vector $\mathbf{a}'$ in the reflection plane but neither along the rotation axis nor perpendicular to it and taking $\mathbf{b}'$ and $\mathbf{c}'$ to be the images of $\mathbf{a}'$ under the threefold rotation and its square. Then the matrices of the threefold rotation and the reflection with respect to the basis $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ are

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

Different choices of a basis for a point group in general result in different matrix groups, and it is natural to consider two point groups as equivalent if they are transformed into each other by a basis transformation. This is entirely analogous to the situation of space groups, where space groups that only differ by the choice of coordinate system are regarded as equivalent. This notion of equivalence is applied at both the level of space groups and point groups.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, are said to belong to the same *geometric crystal class* if $\mathcal{P}$ and $\mathcal{P}'$ become the same matrix group once suitable bases for the three-dimensional space are chosen.

Equivalently, $\mathcal{G}$ and $\mathcal{G}'$ belong to the same geometric crystal class if the point group $\mathcal{P}'$ can be obtained from $\mathcal{P}$ by a basis transformation of the underlying vector space $\mathbb{V}^3$, *i.e.* if there is an invertible 3×3 matrix $\boldsymbol{P}$ such that

$$\mathcal{P}' = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \mid \boldsymbol{W} \in \mathcal{P}\}.$$

Also, two matrix groups $\mathcal{P}$ and $\mathcal{P}'$ are said to belong to the same geometric crystal class if they are conjugate by an invertible 3×3 matrix $\boldsymbol{P}$.

Historically, the geometric crystal classes in dimension 3 were determined much earlier than the space groups. They were obtained as the symmetry groups for the set of normal vectors of crystal faces which describe the morphological symmetry of crystals.

Note that for the geometric crystal classes in dimension 3 (and in all other odd dimensions) the distinction between orientation-preserving and orientation-reversing transformations is irrelevant, since any conjugation by an arbitrary transformation can already be realized by an orientation-preserving transformation. This is due to the fact that the inversion $-\boldsymbol{I}$ on the one hand commutes with every matrix $\boldsymbol{W}$, *i.e.* $(-\boldsymbol{I})\boldsymbol{W} = \boldsymbol{W}(-\boldsymbol{I})$, and on the other hand $\det(-\boldsymbol{I}) = -1$. If $\boldsymbol{P}$ is orientation reversing, one has $\det \boldsymbol{P} < 0$ and then $(-\boldsymbol{I})\boldsymbol{P} = -\boldsymbol{P}$ is orientation preserving because $\det(-\boldsymbol{P}) = -\det \boldsymbol{P} > 0$. But $(-\boldsymbol{P})^{-1}\boldsymbol{W}(-\boldsymbol{P}) = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}$, hence the transformations by $\boldsymbol{P}$ and $-\boldsymbol{P}$ give the same result and one of $\boldsymbol{P}$ and $-\boldsymbol{P}$ is orientation preserving.

Remark: One often speaks of the geometric crystal classes as the *types of point groups*. This emphasizes the point of view in which a point group is regarded as the group of linear parts of a space group, written with respect to an *arbitrary basis* of $\mathbb{R}^n$ (not necessarily a lattice basis).

It is also common to state that *there are 32 point groups in three-dimensional space*. This is just as imprecise as saying that *there are 230 space groups*, since there are in fact infinitely many point groups and space groups.

What is meant when we say that two space groups have *the same point group* is usually that their point groups are of the same type (*i.e.* lie in the same geometric crystal class) and can thus be *made to coincide* by a suitable basis transformation.

Example

In the space group $P3$ the threefold rotation generating the point group is given by the matrix

$$\boldsymbol{W} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

whereas in the space group $R3$ (in the rhombohedral setting) the threefold rotation is given by the matrix

$$\boldsymbol{W}' = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

These two matrices are conjugate by the basis transformation

$$\boldsymbol{P} = \frac{1}{3}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix},$$

which transforms the basis of the hexagonal setting into that of the rhombohedral setting. This shows that the space groups $P3$ and $R3$ belong to the same geometric crystal class.

The example is typical in the sense that different groups in the same geometric crystal class usually describe the same group of linear parts acting on different lattices, *e.g.* primitive and centred. Writing the action of the linear parts with respect to primitive bases of different lattices gives rise to different matrix groups.

1.3.4.3. Bravais types of lattices and Bravais classes

In the classification of space groups into geometric crystal classes, only the point-group part is considered and the translation lattice is ignored. It is natural that the converse point of view is also adopted, where space groups are grouped together according to their translation lattices, irrespective of what the point groups are.

We have already seen that a lattice can be characterized by its metric tensor, containing the scalar products of a primitive basis. If a point group $\mathcal{P}$ acts on a lattice $\mathbf{L}$, it fixes the metric tensor $\boldsymbol{G}$ of $\mathbf{L}$, *i.e.* $\boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}$ for all $\boldsymbol{W}$ in $\mathcal{P}$ and is thus a subgroup of the Bravais group $Aut(\mathbf{L})$ of $\mathbf{L}$. Also, a matrix group $\mathcal{B}$ is called a *Bravais group* if it is the Bravais group $Aut(\mathbf{L})$ for some lattice $\mathbf{L}$. The Bravais groups govern the classification of lattices.

Definition

Two lattices $\mathbf{L}$ and $\mathbf{L}'$ belong to the same *Bravais type of lattices* if their Bravais groups $Aut(\mathbf{L})$ and $Aut(\mathbf{L}')$ are the same matrix group when written with respect to suitable primitive bases of $\mathbf{L}$ and $\mathbf{L}'$.

Note that in order to have the same Bravais group, the metric tensors of the two lattices $\mathbf{L}$ and $\mathbf{L}'$ do not have to be the same or scalings of each other.

Example

The mineral rutile (TiO_2) has a space group of type $P4_2/mnm$ (136) with a primitive tetragonal cell with cell parameters $a = b = 4.594$ Å and $c = 2.959$ Å. The metric tensor of the translation lattice $\mathbf{L}$ is therefore

$$\boldsymbol{G} = \begin{pmatrix} 4.594^2 & 0 & 0 \\ 0 & 4.594^2 & 0 \\ 0 & 0 & 2.959^2 \end{pmatrix}$$

and the Bravais group of the lattice is generated by the fourfold rotation

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

around the z axis, the reflection

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

in the plane $x = 0$ and the reflection

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

in the plane $z = 0$.

The silicate mineral cristobalite also has (at low temperatures) a primitive tetragonal cell with $a = b = 4.971$ Å and $c = 6.928$ Å, and the space-group type is $P4_12_12$ (92). In this case the metric tensor of the translation lattice $\mathbf{L}'$ is

$$\boldsymbol{G}' = \begin{pmatrix} 4.971^2 & 0 & 0 \\ 0 & 4.971^2 & 0 \\ 0 & 0 & 6.928^2 \end{pmatrix}$$

and one checks that the Bravais group of $\mathbf{L}'$ is precisely the same as that of $\mathbf{L}$. Therefore, the translation lattices $\mathbf{L}$ for rutile and $\mathbf{L}'$ for cristobalite belong to the same Bravais type of lattices.

The different Bravais types of lattices, their cell parameters and metric tensors are displayed in Tables 3.1.2.1 (dimension 2) and 3.1.2.2 (dimension 3): in dimension 2 there are 5 Bravais types and in dimension 3 there are 14 Bravais types of lattices.

It is crucial for the classification of lattices *via* their Bravais groups that one works with primitive bases, because a primitive and a body-centred cubic lattice have the same automorphisms when written with respect to the conventional cubic basis, but are clearly different types of lattices.

Example

The silicate mineral zircon ($ZrSiO_4$) has a body-centred tetragonal cell with cell parameters $a = b = 6.607$ Å and $c = 5.982$ Å. The body-centred translation lattice $\mathbf{L}'$ is spanned by the primitive tetragonal lattice $\mathbf{L}$ with basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ with $\alpha = \beta = \gamma = 90^\circ$ and the centring vector $\mathbf{v} = \frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$. A primitive basis of $\mathbf{L}'$ is obtained as $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$ with

$$\boldsymbol{P} = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix},$$

i.e. $\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}) = -\mathbf{a} + \mathbf{v}$, $\mathbf{b}' = \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}) = -\mathbf{b} + \mathbf{v}$, $\mathbf{c}' = \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c}) = -\mathbf{c} + \mathbf{v}$ and the metric tensor $\boldsymbol{G}'$ of $\mathbf{L}'$ with respect to the primitive basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ is

$$\begin{aligned} \boldsymbol{G}' &= \boldsymbol{P}^{\mathrm{T}}\begin{pmatrix} 6.607^2 & 0 & 0 \\ 0 & 6.607^2 & 0 \\ 0 & 0 & 5.982^2 \end{pmatrix}\boldsymbol{P} \\ &= \begin{pmatrix} 5.547^2 & -12.880 & -8.946 \\ -12.880 & 5.547^2 & -8.946 \\ -8.946 & -8.946 & 5.547^2 \end{pmatrix}. \end{aligned}$$

The Bravais group of the primitive tetragonal lattice $\mathbf{L}$ is generated (as in the previous example) by

$$\boldsymbol{W}_1 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{W}_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\text{and } \boldsymbol{W}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and these matrices also generate the Bravais group of the body-centred tetragonal lattice $\mathbf{L}'$, but written with respect to the primitive basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ these matrices are transformed to

$$\boldsymbol{W}_1' = \boldsymbol{P}^{-1}\boldsymbol{W}_1\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{pmatrix},$$

$$\boldsymbol{W}_2' = \boldsymbol{P}^{-1}\boldsymbol{W}_2\boldsymbol{P} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix} \text{ and}$$

$$\boldsymbol{W}_3' = \boldsymbol{P}^{-1}\boldsymbol{W}_3\boldsymbol{P} = \begin{pmatrix} 0 & -1 & 1 \\ -1 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

That the primitive and the body-centred tetragonal lattices have different types ultimately follows from the fact that the body-centred lattice $\mathbf{L}'$ does not have a primitive basis consisting of vectors $\mathbf{a}'', \mathbf{b}'', \mathbf{c}''$ which are pairwise perpendicular and such that $\mathbf{a}''$ and $\mathbf{b}''$ have the same length. This would be required to have the matrices $\boldsymbol{W}_1$, $\boldsymbol{W}_2$ and $\boldsymbol{W}_3$ in the Bravais group of $\mathbf{L}'$.

As we have seen, the metric tensors of lattices belonging to the same Bravais type need not be the same, but if they are written with respect to suitable bases they are found to have the same structure, differing only in the specific values for certain free parameters.

Definition

Let $\mathbf{L}$ be a lattice with metric tensor $\boldsymbol{G}$ with respect to a primitive basis and let $\mathcal{B} = Aut(\mathbf{L}) = \{\boldsymbol{W} \in \mathrm{GL}_3(\mathbb{Z}) \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{W} = \boldsymbol{G}\}$ be the Bravais group of $\mathbf{L}$. Then

$$\mathbf{M}(\mathcal{B}) := \{\boldsymbol{G}' \text{ symmetric } 3 \times 3 \text{ matrix} \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G}' \cdot \boldsymbol{W} = \boldsymbol{G}' \text{ for all } \boldsymbol{W} \in \mathcal{B}\}$$

is called the *space of metric tensors* of $\mathcal{B}$. The dimension of $\mathbf{M}(\mathcal{B})$ is called the *number of free parameters* of the lattice $\mathbf{L}$. Analogously, for an arbitrary integral matrix group $\mathcal{P}$,

$$\mathbf{M}(\mathcal{P}) := \{\boldsymbol{G}' \text{ symmetric } 3 \times 3 \text{ matrix} \mid \boldsymbol{W}^{\mathrm{T}} \cdot \boldsymbol{G}' \cdot \boldsymbol{W} = \boldsymbol{G}' \text{ for all } \boldsymbol{W} \in \mathcal{P}\}$$

is called the *space of metric tensors* of $\mathcal{P}$. If $\dim \mathbf{M}(\mathcal{P}') = \dim \mathbf{M}(\mathcal{P})$ for a subgroup $\mathcal{P}'$ of $\mathcal{P}$, the spaces of metric tensors are the same for both groups and one says that $\mathcal{P}'$ *does not act on a more general lattice* than $\mathcal{P}$ does.

It is clear that $\mathbf{M}(\mathcal{B})$ contains in particular the metric tensor $\boldsymbol{G}$ of the lattice $\mathbf{L}$ of which $\mathcal{B}$ is the Bravais group. Moreover, $\mathcal{B}$ is a subgroup of the Bravais group of every lattice with metric tensor in $\mathbf{M}(\mathcal{B})$.

Example

Let **L** be a lattice with metric tensor

$$\begin{pmatrix} 17 & 0 & 0 \\ 0 & 17 & 0 \\ 0 & 0 & 42 \end{pmatrix},$$

then **L** is a tetragonal lattice with Bravais group $\mathcal{B}$ of type 4/*mmm* generated by the fourfold rotation

$$\boldsymbol{W}_1 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the reflections

$$\boldsymbol{W}_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \boldsymbol{W}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The space of metric tensors of $\mathcal{B}$ is

$$\mathbf{M}(\mathcal{B}) = \left\{ \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{11} & 0 \\ 0 & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{33} \in \mathbb{R} \right\}$$

and the number of free parameters of **L** is 2.

For every lattice $\mathbf{L}'$ with metric tensor $\boldsymbol{G}'$ in $\mathbf{M}(\mathcal{B})$ such that $g_{11} \neq g_{33}$, one can check that the Bravais group of $\mathbf{L}'$ is equal to $\mathcal{B}$, hence these lattices belong to the same Bravais type of lattices as **L**. On the other hand, if it happens that $g_{11} = g_{33}$ in the metric tensor $\boldsymbol{G}'$ of a lattice $\mathbf{L}'$, then the Bravais group of $\mathbf{L}'$ is the full cubic point group of type $m\bar{3}m$ and $\mathcal{B}$ is a proper subgroup of the Bravais group of $\mathbf{L}'$. In this case the lattice $\mathbf{L}'$ is of a different Bravais type to **L**, namely cubic.

The subgroup $\mathcal{P}$ of $\mathcal{B}$ generated only by the fourfold rotation $\boldsymbol{W}_1$ has the same space of metric tensors as $\mathcal{B}$, thus this subgroup acts on the same types of lattices as $\mathcal{B}$ (*i.e.* tetragonal lattices). On the other hand, for the subgroup $\mathcal{P}'$ of $\mathcal{B}$ generated by the reflections $\boldsymbol{W}_2$ and $\boldsymbol{W}_3$, the space of metric tensors is

$$\mathbf{M}(\mathcal{P}') = \left\{ \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{22}, g_{33} \in \mathbb{R} \right\}$$

and is thus of dimension 3. This shows that the subgroup $\mathcal{P}'$ acts on more general lattices than $\mathcal{B}$, namely on orthorhombic lattices.

Remark: The metric tensor of a lattice basis is a *positive definite*[2] matrix. It is clear that not all matrices in $\mathbf{M}(\mathcal{B})$ are positive definite [if $\boldsymbol{G} \in \mathbf{M}(\mathcal{B})$ is positive definite, then $-\boldsymbol{G}$ is certainly not positive definite], but the different geometries of lattices on which $\mathcal{B}$ acts are represented precisely by the positive definite metric tensors in $\mathbf{M}(\mathcal{B})$.

The space of metric tensors obtained from a lattice can be interpreted as an expression of the metric tensor with general entries, *i.e.* as a generic metric tensor describing the different lattices within the same Bravais type. Special choices for the entries may lead to lattices with accidental higher symmetry, which is in fact a common phenomenon in phase transitions caused by changes of temperature or pressure.

One says that the translation lattice **L** of a space group $\mathcal{G}$ with point group $\mathcal{P}$ has a *specialized metric* if the dimension of the space of metric tensors of $\mathcal{B} = Aut(\mathbf{L})$ is smaller than the dimension of the space of metric tensors of $\mathcal{P}$. Viewed from a slightly different angle, a specialized metric occurs if the location of the atoms within the unit cell reduces the symmetry of the translation lattice to that of a different lattice type.

Example

A space group $\mathcal{G}$ of type $P2/m$ (10) with cell parameters $a = 4.4$, $b = 5.5$, $c = 6.6$ Å, $\alpha = \beta = \gamma = 90^\circ$ has a specialized metric, because the point group $\mathcal{P}$ of type $2/m$ is generated by

$$\boldsymbol{W} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and $-\boldsymbol{I}$, and has

$$\mathbf{M}(\mathcal{P}) = \left\{ \begin{pmatrix} g_{11} & 0 & g_{13} \\ 0 & g_{22} & 0 \\ g_{13} & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{22}, g_{33}, g_{13} \in \mathbb{R} \right\}$$

as its space of metric tensors, which is of dimension 4. The lattice **L** with the given cell parameters, however, is orthorhombic, since the free parameter g_{13} is specialized to $g_{13} = 0$. The automorphism group $Aut(\mathbf{L})$ is of type *mmm* and has a space of metric tensors of dimension 3, namely

$$\left\{ \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix} \mid g_{11}, g_{22}, g_{33} \in \mathbb{R} \right\}.$$

The higher symmetry of the translation lattice would, for example, be destroyed by an atomic configuration compatible with the lattice and represented by only two atoms in the unit cell located at 0.17, 1/2, 0.42 and 0.83, 1/2, 0.58. The two atoms are related by a twofold rotation around the *b* axis, which indicates the invariance of the configuration under twofold rotations with axes parallel to **b**, but in contrast to the lattice **L**, the atomic configuration is not compatible with rotations around the *a* or the *c* axes.

By looking at the spaces of metric tensors, space groups can be classified according to the Bravais types of their translation lattices, without suffering from complications due to specialized metrics.

Definition

Let **L** be a lattice with metric tensor $\boldsymbol{G}$ and Bravais group $\mathcal{B} = Aut(\mathbf{L})$ and let $\mathbf{M}(\mathcal{B})$ be the space of metric tensors associated to **L**. Then those space groups $\mathcal{G}$ form the *Bravais class* corresponding to the Bravais type of **L** for which $\mathbf{M}(\mathcal{P}) = \mathbf{M}(\mathcal{B})$ when the point group $\mathcal{P}$ of $\mathcal{G}$ is written with respect to a suitable primitive basis of the translation lattice of $\mathcal{G}$. The names for the Bravais classes are the same as those for the corresponding Bravais types of lattices.

The Bravais groups of lattices provide a link between lattices and point groups, the two building blocks of space groups. However, although the Bravais group of a lattice is simply a matrix group, the fact that it is expressed with respect to a primitive basis and fixes the metric tensor of the lattice preserves the necessary information about the lattice. When the Bravais group is regarded as a point group, the information about the lattice is lost, since point groups can be written with respect to an arbitrary basis. In order to distinguish Bravais groups of lattices at the level of point groups and geometric crystal classes, the concept of a holohedry is introduced.

[2] A symmetric matrix $\boldsymbol{G}$ is *positive definite* if $\mathbf{v}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \mathbf{v} > 0$ for every vector $\mathbf{v} \neq 0$.

Definition

The geometric crystal class of a point group $\mathcal{P}$ is called a *holohedry* (or *lattice point group*, *cf.* Chapters 3.1 and 3.3) if $\mathcal{P}$ is the Bravais group of some lattice **L**.

Example

Let $\mathcal{P}$ be the point group of type $\bar{3}m$ generated by the threefold rotoinversion

$$\boldsymbol{W}_1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

around the z axis and the twofold rotation

$$\boldsymbol{W}_2 = \begin{pmatrix} 1 & -1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

expressed with respect to the conventional basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of a hexagonal lattice. The group $\mathcal{P}$ is not the Bravais group of the lattice **L** spanned by $\mathbf{a}, \mathbf{b}, \mathbf{c}$ because this lattice also allows a sixfold rotation around the z axis, which is not contained in $\mathcal{P}$. But $\mathcal{P}$ also acts on the rhombohedrally centred lattice $\mathbf{L}'$ with primitive basis $\mathbf{a}' = \frac{1}{3}(2\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + \mathbf{b} + \mathbf{c})$, $\mathbf{c}' = \frac{1}{3}(-\mathbf{a} - 2\mathbf{b} + \mathbf{c})$. With respect to the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ the rotoinversion and twofold rotation are transformed to

$$\boldsymbol{W}_1' = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \text{ and } \boldsymbol{W}_2' = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

and these matrices indeed generate the Bravais group of $\mathbf{L}'$. The geometric crystal class with symbol $\bar{3}m$ is therefore a holohedry.

Note that in dimension 3 the above is actually the only example of a geometric crystal class in which the point groups are Bravais groups for some but not for all the lattices on which they act. In all other cases, each matrix group $\mathcal{P}$ corresponding to a holohedry is actually the Bravais group of the lattice spanned by the basis with respect to which $\mathcal{P}$ is written.

1.3.4.4. Other classifications of space groups

In this section we summarize a number of other classification schemes which are perhaps of slightly lower significance than those of space-group types, geometric crystal classes and Bravais types of lattices, but also play an important role for certain applications.

1.3.4.4.1. Arithmetic crystal classes

We have already seen that every space group can be assigned to a symmorphic space group in a natural way by setting the translation parts of coset representatives with respect to the translation subgroup to $\boldsymbol{o}$. The groups assigned to a symmorphic space group in this way all have the same translation lattice and the same point group but the different possibilities for the interplay between these two parts are ignored.

If we want to collect together all space groups that correspond to symmorphic space groups of the same type, we arrive at the classification into *arithmetic crystal classes*. This can also be seen as a classification of the symmorphic space-group types. The distribution of the space groups into arithmetic classes, represented by the corresponding symmorphic space-group types, is given in Table 2.1.3.3.

The crucial observation for characterizing this classification is that space groups that correspond to the same symmorphic space group all have translation lattices of the same Bravais type. This means that the freedom in the choice of a basis transformation of the underlying vector space is restricted, because a primitive basis has to be mapped again to a primitive basis. Assuming that the point groups are written with respect to primitive bases, this means that the basis transformation is an integral matrix with determinant ± 1.

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, both written with respect to primitive bases of their translation lattices, are said to lie in the same *arithmetic crystal class* if $\mathcal{P}'$ can be obtained from $\mathcal{P}$ by an integral basis transformation of determinant ± 1, *i.e.* if there is an integral 3×3 matrix $\boldsymbol{P}$ with $\det \boldsymbol{P} = \pm 1$ such that

$$\mathcal{P}' = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \mid \boldsymbol{W} \in \mathcal{P}\}.$$

Also, two integral matrix groups $\mathcal{P}$ and $\mathcal{P}'$ are said to belong to the same arithmetic crystal class if they are conjugate by an integral 3×3 matrix $\boldsymbol{P}$ with $\det \boldsymbol{P} = \pm 1$.

Example

Let

$$\boldsymbol{M}_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{M}_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\text{and } \boldsymbol{M}_3 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

be reflections in the planes $x = 0$, $y = 0$ and $x = y$, respectively, and let $\mathcal{P}_1 = \langle \boldsymbol{M}_1 \rangle$, $\mathcal{P}_2 = \langle \boldsymbol{M}_2 \rangle$ and $\mathcal{P}_3 = \langle \boldsymbol{M}_3 \rangle$ be the integral matrix groups generated by these reflections. Then $\mathcal{P}_1$ and $\mathcal{P}_2$ belong to the same arithmetic crystal class because they are transformed into each other by the basis transformation

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

interchanging the x and y axes. But $\mathcal{P}_3$ belongs to a different arithmetic crystal class, because $\boldsymbol{M}_3$ is not conjugate to $\boldsymbol{M}_1$ by an integral matrix $\boldsymbol{P}$ of determinant ± 1. The two groups $\mathcal{P}_1$ and $\mathcal{P}_3$ belong, however, to the same geometric crystal class, because $\boldsymbol{M}_1$ and $\boldsymbol{M}_3$ are transformed into each other by the basis transformation

$$\boldsymbol{P} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

which has determinant $\frac{1}{2}$. This basis transformation shows that $\boldsymbol{M}_1$ and $\boldsymbol{M}_3$ can be interpreted as the action of the same reflection on a primitive lattice and on a C-centred lattice.

As explained above, the number of arithmetic crystal classes is equal to the number of symmorphic space-group types: in dimension 2 there are 13 such classes, in dimension 3 there are 73 arithmetic crystal classes. The Hermann–Mauguin symbol of the symmorphic space-group type to which a space group $\mathcal{G}$ belongs is obtained from the symbol for the space-group type of $\mathcal{G}$ by replacing any screw-rotation axis symbol N_m by the corre-

sponding rotation axis symbol N and every glide-plane symbol a, b, c, d, e, n by the symbol m for a mirror plane.

It is clear that the classification into arithmetic crystal classes refines both the classifications into geometric crystal classes and into Bravais classes, since in the first case only the point groups and in the second case only the translation lattices are taken into account, whereas for the arithmetic crystal classes the combination of point groups and translation lattices is considered. Note, however, that for the determination of the arithmetic crystal class of a space group $\mathcal{G}$ it is not sufficient to look only at the type of the point group and the Bravais type of the translation lattice. It is crucial to consider the action of the point group on the translation lattice.

Example

Let $\mathcal{G}$ and $\mathcal{G}'$ be space groups of types $P3m1$ (156) and $P31m$ (157), respectively. Since $\mathcal{G}$ and $\mathcal{G}'$ are symmorphic space groups of different types, they must belong to different arithmetic classes. The point groups $\mathcal{P}$ and $\mathcal{P}'$ of $\mathcal{G}$ and $\mathcal{G}'$ both belong to the same geometric crystal class with symbol $3m$ and the translation lattices of both space groups are primitive hexagonal lattices, and thus of the same Bravais type. It is the different action on the translation lattice which causes $\mathcal{G}$ and $\mathcal{G}'$ to lie in different arithmetic classes:

In the conventional setting, the point group $\mathcal{P}$ of $\mathcal{G}$ contains the threefold rotation

$$\boldsymbol{R} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the reflections

$$\boldsymbol{M}_1 = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{M}_2 = \begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\text{and } \boldsymbol{M}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

whereas the point group $\mathcal{P}'$ of $\mathcal{G}'$ contains the same rotation $\boldsymbol{R}$ and the reflections

$$\boldsymbol{M}'_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \boldsymbol{M}'_2 = \begin{pmatrix} 1 & -1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\text{and } \boldsymbol{M}'_3 = \begin{pmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Since the threefold rotation is represented by the same matrix in both groups, the lattice basis for both groups can be taken as the conventional basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ of a hexagonal lattice, with $\mathbf{a}$ and $\mathbf{b}$ of the same length and enclosing an angle of 120° and $\mathbf{c}$ perpendicular to the plane spanned by $\mathbf{a}$ and $\mathbf{b}$. One now sees that in $\mathcal{P}'$ the reflection planes of $\boldsymbol{M}'_1$, $\boldsymbol{M}'_2$ and $\boldsymbol{M}'_3$ contain the vectors $\mathbf{a}+\mathbf{b}$, $\mathbf{a}$ and $\mathbf{b}$, respectively, whereas in $\mathcal{P}$ these vectors are just perpendicular to the reflection planes. In the so-called hexagonally centred lattice with primitive basis $\mathbf{a}' = \frac{1}{3}\mathbf{a} + \frac{2}{3}\mathbf{b}$, $\mathbf{b}' = -\frac{2}{3}\mathbf{a} - \frac{1}{3}\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, the vectors $\mathbf{a}'$ and $\mathbf{b}'$ are perpendicular to the vectors $\mathbf{a}$ and $\mathbf{b}$. The group $\mathcal{G}'$ can thus be regarded as the action of $\mathcal{G}$ on the hexagonally centred lattice, showing that $\mathcal{G}$ and $\mathcal{G}'$ are actions of the same group on different lattices which therefore belong to different arithmetic crystal classes.

As we have seen, the assignment of a space group to its arithmetic crystal class is equivalent to the assignment to its corresponding symmorphic space group, which in turn can be seen as an assignment to the combination of a point group and a lattice on which this point group acts. This correspondence between arithmetic crystal classes and point group/lattice combinations is reflected in the symbol for an arithmetic crystal class suggested in de Wolff *et al.* (1985), which is the symbol of the symmorphic space group with the letter for the lattice moved to the end, *e.g.* $4mmP$ for the arithmetic crystal class containing the symmorphic space groups of type $P4mm$ (99) and the non-symmorphic groups derived from this symmorphic group, *i.e.* the groups of space-group type $P4bm$, $P4_2cm$, $P4_2nm$, $P4cc$, $P4nc$, $P4_2mc$ and $P4_2bc$ (100–106).

Recall that the members of one arithmetic crystal class are space groups with the same translation lattice and the same point group, possibly written with respect to different primitive bases. If the point group happens to be the Bravais group of the translation lattice, this is independent of the chosen primitive basis and thus being a Bravais group is clearly a property of the full arithmetic crystal class.

Definition

The arithmetic crystal class of a space group $\mathcal{G}$ is called a *Bravais arithmetic crystal class* if the point group of $\mathcal{G}$ is the Bravais group of the translation lattice of $\mathcal{G}$.

The arithmetic crystal class of an integral matrix group $\mathcal{P}$ is a Bravais arithmetic crystal class if $\mathcal{P}$ is maximal among the integral matrix groups with the same space of metric tensors $\mathbf{M}(\mathcal{P})$, *i.e.* if for any integral matrix group $\mathcal{P}'$ properly containing $\mathcal{P}$ as a subgroup, the space of metric tensors $\mathbf{M}(\mathcal{P}')$ is strictly smaller than that of $\mathcal{P}$. This amounts to saying that $\mathcal{P}'$ must act on a lattice with specialized metric.

Note that in the previous edition of *IT* A the shorter term *Bravais class* was used as a synonym for Bravais arithmetic crystal class. However, in this edition the term *Bravais class* is reserved for the classification of space-group types according to their lattices (see Section 1.3.4.3).

Since the lattice types are characterized by their Bravais groups, the Bravais arithmetic crystal classes are in one-to-one correspondence with the Bravais types of lattices. The 14 Bravais arithmetic crystal classes (given by the symbol for the arithmetic class, with the number of the associated symmorphic space-group type in brackets) and the corresponding lattice types are: $\bar{1}P$ (2), triclinic; $2/mP$ (10), primitive monoclinic; $2/mC$ (12), centred monoclinic; $mmmP$ (47), primitive orthorhombic; $mmmC$ (65), single-face-centred orthorhombic; $mmmF$ (69), all-face-centred orthorhombic; $mmmI$ (71), body-centred orthorhombic; $4/mmmP$ (123), primitive tetragonal; $4/mmmI$ (139), body-centred tetragonal; $\bar{3}mR$ (166), rhombohedral; $6/mmmP$ (191), hexagonal; $m\bar{3}mP$ (221), primitive cubic; $m\bar{3}mF$ (225), face-centred cubic; and $m\bar{3}mI$ (229), body-centred cubic.

Bravais flocks

In the classification of space groups according to their translation lattices, the point groups play only a secondary role (as groups acting on the lattices). From the perspective of arithmetic crystal classes, this classification can now be reformulated in terms of integral matrix groups. The crucial point is that every arithmetic crystal class can be assigned to a Bravais arithmetic crystal class in a natural way: If $\mathcal{P}$ is a point group, there is a

Table 1.3.4.1
Lattice systems in three-dimensional space

Lattice system	Bravais types of lattices	Holohedry
Triclinic (anorthic)	*aP*	$\bar{1}$
Monoclinic	*mP*, *mS*	2/*m*
Orthorhombic	*oP*, *oS*, *oF*, *oI*	*mmm*
Tetragonal	*tP*, *tI*	4/*mmm*
Hexagonal	*hP*	6/*mmm*
Rhombohedral	*hR*	$\bar{3}m$
Cubic	*cP*, *cF*, *cI*	$m\bar{3}m$

Table 1.3.4.2
Crystal systems in three-dimensional space

Crystal system	Point-group types
Triclinic	$\bar{1}$, 1
Monoclinic	2/*m*, *m*, 2
Orthorhombic	*mmm*, *mm*2, 222
Tetragonal	4/*mmm*, $\bar{4}2m$, 4*mm*, 422, 4/*m*, $\bar{4}$, 4
Hexagonal	6/*mmm*, $\bar{6}2m$, 6*mm*, 622, 6/*m*, $\bar{6}$, 6
Trigonal	$\bar{3}m$, 3*m*, 32, $\bar{3}$, 3
Cubic	$m\bar{3}m$, $\bar{4}3m$, 432, $m\bar{3}$, 23

unique Bravais arithmetic crystal class containing a Bravais group $\mathcal{B}$ of minimal order with $\mathcal{P} \leq \mathcal{B}$. Conversely, a Bravais group $\mathcal{B}$ acting on a lattice **L** is grouped together with its subgroups $\mathcal{P}$ that do not act on a more general lattice, *i.e.* on a lattice **L**′ with more free parameters than **L**. This observation gives rise to the concept of *Bravais flocks*, which is mainly applied to matrix groups.

Definition

Two integral matrix groups $\mathcal{P}$ and $\mathcal{P}'$ belong to the same Bravais flock if they are both conjugate by an integral basis transformation to subgroups of a common Bravais group, *i.e.* if there exists a Bravais group $\mathcal{B}$ and integral 3×3 matrices $\boldsymbol{P}$ and $\boldsymbol{P}'$ such that $\boldsymbol{PWP}^{-1} \in \mathcal{B}$ for all $\boldsymbol{W} \in \mathcal{P}$ and $\boldsymbol{P}'\boldsymbol{W}'\boldsymbol{P}'^{-1} \in \mathcal{B}$ for all $\boldsymbol{W}' \in \mathcal{P}'$. Moreover, $\mathcal{P}$, $\mathcal{P}'$ and $\mathcal{B}$ must all have spaces of metric tensors of the same dimension.

Each Bravais flock consists of the union of the arithmetic crystal class of a Bravais group $\mathcal{B}$ and the arithmetic crystal classes of the subgroups of $\mathcal{B}$ that do not act on a more general lattice than $\mathcal{B}$.

The classification of space groups into Bravais flocks is the same as that according to the Bravais types of lattices and as that into Bravais classes. If the point groups $\mathcal{P}$ and $\mathcal{P}'$ of two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same Bravais flock, then the space groups are also said to belong to the same Bravais flock, but this is the case if and only if $\mathcal{G}$ and $\mathcal{G}'$ belong to the same Bravais class.

Example

For the body-centred tetragonal lattice the Bravais arithmetic crystal class is the arithmetic crystal class 4/*mmmI* and the corresponding symmorphic space-group type is *I*4/*mmm* (139). The other arithmetic crystal classes in this Bravais flock are (with the number of the corresponding symmorphic space group in brackets): 4*I* (79), $\bar{4}I$ (82), 4/*mI* (87), 422*I* (97), 4*mmI* (107), $\bar{4}m2I$ (119) and $\bar{4}2mI$ (121).

1.3.4.4.2. Lattice systems

It is sometimes convenient to group together those Bravais types of lattices for which the Bravais groups belong to the same holohedry.

Definition

Two lattices belong to the same *lattice system* if their Bravais groups belong to the same geometric crystal class (which is thus a holohedry).

Remark: The lattice systems were called *Bravais systems* in earlier editions of this volume.

Example

The primitive cubic, face-centred cubic and body-centred cubic lattices all belong to the same lattice system, because their Bravais groups all belong to the holohedry with symbol $m\bar{3}m$.

On the other hand, the hexagonal and the rhombohedral lattices belong to different lattice systems, because their Bravais groups are not even of the same order and lie in different holohedries (with symbols 6/*mmm* and $\bar{3}m$, respectively).

From the definition it is obvious that lattice systems classify lattices because they consist of full Bravais types of lattices. On the other hand, the example of the geometric crystal class $\bar{3}m$ shows that lattice systems do not classify point groups, because depending on the chosen basis a point group in this geometric crystal class belongs to either the hexagonal or the rhombohedral lattice system.

However, since the translation lattices of space groups in the same Bravais class belong to the same Bravais type of lattices, the lattice systems can also be regarded as a classification of space groups in which full Bravais classes are grouped together.

Definition

Two Bravais classes belong to the same *lattice system* if the corresponding Bravais arithmetic crystal classes belong to the same holohedry.

More precisely, two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same lattice system if the point groups $\mathcal{P}$ and $\mathcal{P}'$ are contained in Bravais groups $\mathcal{B}$ and $\mathcal{B}'$, respectively, such that $\mathcal{B}$ and $\mathcal{B}'$ belong to the same holohedry and such that $\mathcal{P}$, $\mathcal{P}'$, $\mathcal{B}$ and $\mathcal{B}'$ all have spaces of metric tensors of the same dimension.

Every lattice system contains the lattices of precisely one holohedry and a holohedry determines a unique lattice system, containing the lattices of the Bravais arithmetic crystal classes in the holohedry. Therefore, there is a one-to-one correspondence between holohedries and lattice systems. There are four lattice systems in dimension 2 and seven lattice systems in dimension 3. The lattice systems in three-dimensional space are displayed in Table 1.3.4.1. Along with the name of each lattice system, the Bravais types of lattices contained in it and the corresponding holohedry are given.

1.3.4.4.3. Crystal systems

The point groups contained in a geometric crystal class can act on different Bravais types of lattices, which is the reason why lattice systems do not classify point groups. But the action on different types of lattices can be exploited for a classification of point groups by joining those geometric crystal classes that act on the same Bravais types of lattices. For example, the holohedry $m\bar{3}m$ acts on primitive, face-centred and body-centred cubic lattices. The other geometric crystal classes that act on these three types of lattices are 23, $m\bar{3}$, 432 and $\bar{4}3m$.

Table 1.3.4.3
Distribution of space-group types in the hexagonal crystal family

Crystal system	Geometric crystal class	Lattice system	
		Hexagonal	Rhombohedral
Hexagonal	6/*mmm* $\bar{6}2m$ 6*mm* 622 6/*m* $\bar{6}$ 6	*P*6/*mmm*, *P*6/*mcc*, $P6_3/mcm$, $P6_3/mmc$ $P\bar{6}m2$, $P\bar{6}c2$, $P\bar{6}2m$, $P\bar{6}2c$ *P*6*mm*, *P*6*cc*, $P6_3cm$, $P6_3mc$ *P*622, $P6_122$, $P6_522$, $P6_222$, $P6_422$, $P6_322$ *P*6/*m*, $P6_3/m$ $P\bar{6}$ *P*6, $P6_1$, $P6_5$, $P6_2$, $P6_4$, $P6_3$	
Trigonal	$\bar{3}m$ 3*m* 32 $\bar{3}$ 3	$P\bar{3}1m$, $P\bar{3}1c$, $P\bar{3}m1$, $P\bar{3}c1$ *P*3*m*1, *P*31*m*, *P*3*c*1, *P*31*c* *P*312, *P*321, $P3_112$, $P3_121$, $P3_212$, $P3_221$ $P\bar{3}$ *P*3, $P3_1$, $P3_2$	$R\bar{3}m$, $R\bar{3}c$ *R*3*m*, *R*3*c* *R*32 $R\bar{3}$ *R*3

Definition

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, belong to the same *crystal system* if the sets of Bravais types of lattices on which $\mathcal{P}$ and $\mathcal{P}'$ act coincide. Since point groups in the same geometric crystal class act on the same types of lattices, crystal systems consist of full geometric crystal classes and the point groups $\mathcal{P}$ and $\mathcal{P}'$ are also said to belong to the same crystal system.

Remark: In the literature there are many different notions of crystal systems. In *International Tables*, only the one defined above is used.

In many cases, crystal systems collect together geometric crystal classes for point groups that are in a group–subgroup relation and act on lattices with the same number of free parameters. However, this condition is not sufficient. If a point group $\mathcal{P}$ is a subgroup of another point group $\mathcal{P}'$, it is clear that $\mathcal{P}$ acts on each lattice on which $\mathcal{P}'$ acts. But $\mathcal{P}$ may in addition act on different types of lattices on which $\mathcal{P}'$ does not act.

Note that it is sufficient to consider the action on lattices with the maximal number of free parameters, since the action on these lattices implies the action on lattices with a smaller number of free parameters (corresponding to metric specializations).

Example

The holohedry of type 4/*mmm* acts on tetragonal and body-centred tetragonal lattices. The crystal system containing this holohedry thus consists of all the geometric crystal classes in which the point groups act on tetragonal and body-centred tetragonal lattices, but not on lattices with more than two free parameters. This is the case for all geometric crystal classes with point groups containing a fourfold rotation or rotoinversion and that are subgroups of a point group of type 4/*mmm*. This means that the crystal system containing the holohedry 4/*mmm* consists of the geometric classes of types 4, $\bar{4}$, 4/*m*, 422, 4*mm*, $\bar{4}2m$ and 4/*mmm*.

This example is typical for the situation in three-dimensional space, since in three-dimensional space usually all the arithmetic crystal classes contained in a holohedry are Bravais arithmetic crystal classes. In this case, the geometric crystal classes in the crystal system of the holohedry are simply the classes of those subgroups of a point group in the holohedry that do not act on lattices with a larger number of free parameters.

The only exceptions from this situation are the Bravais arithmetic crystal classes for the hexagonal and rhombohedral lattices.

Example

A point group containing a threefold rotation but no sixfold rotation or rotoinversion acts both on a hexagonal lattice and on a rhombohedral lattice. On the other hand, point groups containing a sixfold rotation only act on a hexagonal but not on a rhombohedral lattice. The geometric crystal classes of point groups containing a threefold rotation or rotoinversion but not a sixfold rotation or rotoinversion form a crystal system which is called the *trigonal crystal system*. The geometric crystal classes of point groups containing a sixfold rotation or rotoinversion form a different crystal system, which is called the *hexagonal crystal system*.

The classification of the point-group types into crystal systems is summarized in Table 1.3.4.2.

Remark: Crystal systems can contain at most one holohedry and in dimensions 2 and 3 it is true that every crystal system does contain a holohedry. However, this is not true in higher dimensions. The smallest counter-examples exist in dimension 5, where two (out of 59) crystal systems do not contain any holohedry.

1.3.4.4.4. Crystal families

The classification into crystal systems has many important applications, but it has the disadvantage that it is not compatible with the classification into lattice systems. Space groups that belong to the hexagonal lattice system are distributed over the trigonal and the hexagonal crystal system. Conversely, space groups in the trigonal crystal system belong to either the rhombohedral or the hexagonal lattice system. It is therefore desirable to define a further classification level in which the classes consist of full crystal systems and of full lattice systems, or, equivalently, of full geometric crystal classes and full Bravais classes. Since crystal systems already contain only geometric crystal classes with spaces of metric tensors of the same dimension, this can be achieved by the following definition.

Definition

For a space group $\mathcal{G}$ with point group $\mathcal{P}$ the *crystal family* of $\mathcal{G}$ is the union of all geometric crystal classes that contain a space group $\mathcal{G}'$ that has the same Bravais type of lattices as $\mathcal{G}$.

The crystal family of $\mathcal{G}$ thus consists of those geometric crystal classes that contain a point group $\mathcal{P}'$ such that $\mathcal{P}$ and $\mathcal{P}'$ are contained in a common supergroup $\mathcal{B}$ (which is a Bravais group) and such that $\mathcal{P}$, $\mathcal{P}'$ and $\mathcal{B}$ all act on lattices with the same number of free parameters.

In two-dimensional space, the crystal families coincide with the crystal systems and in three-dimensional space only the trigonal and hexagonal crystal system are merged into a single crystal family, whereas all other crystal systems again form a crystal family on their own.

Example

The trigonal and hexagonal crystal systems belong to a single crystal family, called the *hexagonal crystal family*, because for both crystal systems the number of free parameters of the corresponding lattices is 2 and a point group of type $\bar{3}m$ in the trigonal crystal system is a subgroup of a point group of type 6/*mmm* in the hexagonal crystal system.

A space group in the hexagonal crystal family belongs to either the trigonal or the hexagonal crystal system and to either the rhombohedral or the hexagonal lattice system. A group in the hexagonal crystal system cannot belong to the rhombohedral lattice system, but all other combinations of crystal system and lattice system are possible. The distribution of the space groups in the hexagonal crystal family over these different combinations is displayed in Table 1.3.4.3.

Remark: Up to dimension 3 it seems exceptional that a crystal family contains more than one crystal system, since the only instance of this phenomenon is the hexagonal crystal family consisting of the trigonal and the hexagonal crystal systems. However, in higher dimensions it actually becomes rare that a crystal family consists only of a single crystal system.

For the space groups within one crystal family the same coordinate system is usually used, which is called the *conventional coordinate system* (for this crystal family). However, depending on the application it may be useful to work with a different coordinate system. To avoid confusion, it is recommended to state explicitly when a coordinate system differing from the conventional coordinate system is used.

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1.4. Space groups and their descriptions

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1.4.1. Symbols of space groups

By H. Wondratschek

1.4.1.1. Introduction

Space groups describe the symmetries of crystal patterns; the point group of the space group is the symmetry of the macroscopic crystal. Both kinds of symmetry are characterized by symbols of which there are different kinds. In this section the space-group numbers as well as the Schoenflies symbols and the Hermann–Mauguin symbols of the space groups and point groups will be dealt with and compared, because these are used throughout this volume. They are rather different in their aims. For the Fedorov symbols, mainly used in Russian crystallographic literature, *cf.* Chapter 3.3. In that chapter the Hermann–Mauguin symbols and their use are also discussed in detail. For computer-adapted symbols of space groups implemented in crystallographic software, such as *Hall symbols* (Hall, 1981*a*,*b*) or *explicit symbols* (Shmueli, 1984), the reader is referred to Chapter 1.4 of *International Tables for Crystallography*, Volume B (2008).

For the definition of space groups and plane groups, *cf.* Chapter 1.3. The plane groups characterize the symmetries of two-dimensional periodic arrangements, realized in sections and projections of crystal structures or by periodic wallpapers or tilings of planes. They are described individually and in detail in Chapter 2.2. Groups of one- and two-dimensional periodic arrangements embedded in two-dimensional and three-dimensional space are called *subperiodic groups*. They are listed in Vol. E of *International Tables for Crystallography* (2010) (referred to as *IT* E) with symbols similar to the Hermann–Mauguin symbols of plane groups and space groups, and are related to these groups as their subgroups. The space groups *sensu stricto* are the symmetries of periodic arrangements in three-dimensional space, *e.g.* of normal crystals, see also Chapter 1.3. They are described individually and in detail in the space-group tables of Chapter 2.3. In the following, if not specified separately, both space groups and plane groups are covered by the term *space group*.

The description of each space group in the tables of Chapter 2.3 starts with two headlines in which the different symbols of the space group are listed. All these names are explained in this section with the exception of the data for *Patterson symmetry* (*cf.* Chapter 1.6 and Section 2.1.3.5 for explanations of Patterson symmetry).

1.4.1.2. Space-group numbers

The space-group numbers were introduced in *International Tables for X-ray Crystallography* (1952) [referred to as *IT* (1952)] for plane groups (Nos. 1–17) and space groups (Nos. 1–230). They provide a short way of specifying the type of a space group uniquely, albeit without reference to its symmetries. They are particularly convenient for use with computers and have been in use since their introduction.

There are no numbers for the point groups.

1.4.1.3. Schoenflies symbols

The Schoenflies symbols were introduced by Schoenflies (1891, 1923). They describe the point-group type, also known as the geometric crystal class or (for short) crystal class (*cf.* Section 1.3.4.2), of the space group geometrically. The different space-group types within the same crystal class are denoted by a superscript index appended to the point-group symbol.

1.4.1.3.1. Schoenflies symbols of the crystal classes

Schoenflies derived the point groups as groups of crystallographic symmetry operations, but described these crystallographic point groups geometrically by their representation through axes of rotation or rotoreflection and reflection planes (also called mirror planes), *i.e.* by *geometric elements*; for geometric elements of symmetry elements, *cf.* Section 1.2.3, de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000). Rotation axes dominate the description and planes of reflection are added when necessary. Rotoreflection axes are also indicated when necessary. The orientation of a reflection plane, whether *horizontal*, *vertical* or *diagonal*, refers to the plane itself, not to its normal.

A coordinate basis may be chosen by the user: the basis vectors start at the origin which is placed in front of the user. The basis vector **c** points vertically upwards, the basis vectors **a** and **b** lie

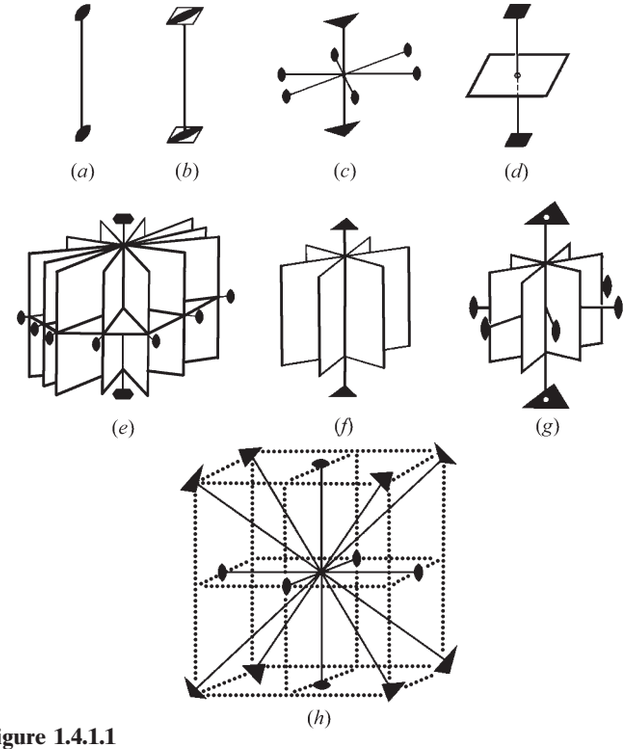

Figure 1.4.1.1
Symmetry-element diagrams of some point groups [adapted from Vainshtein (1994)]. The point groups are specified by their Schoenflies and Hermann–Mauguin symbols. (*a*) $C_2 = 2$, (*b*) $S_4 = \bar{4}$, (*c*) $D_3 = 32$, (*d*) $C_{4h} = 4/m$, (*e*) $D_{6h} = 6/m\,2/m\,2/m$, (*f*) $C_{3v} = 3m$, (*g*) $D_{3d} = \bar{3}\,2/m$, (*h*) $T = 23$. [The cubic frame in part (*h*) has no crystallographic meaning: it has been included to aid visualization of the orientation of the symmetry elements.]

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more or less horizontal; the basis vector **a** pointing at the user, **b** pointing to the user's right-hand side, *i.e.* the basis vectors **a**, **b** and **c** form a *right-handed* set. Such a basis will be called a *conventional crystallographic basis* in this chapter. (In the usual basis of mathematics and physics the basis vector **a** points to the right-hand side and **b** points away from the user.) The lengths of the basis vectors, the inclination of the **ab** plane relative to the **c** axis and the angles between the basis vectors are determined by the symmetry of the point group and the specific values of the lattice parameters of the crystal structure.

The letter C is used for *cyclic groups* of rotations around a rotation axis which is conventionally **c**. The order n of the rotation is appended as a subscript index: C_n; Fig. 1.4.1.1(a) represents C_2. The values of n that are possible in the rotation symmetry of a crystal are 1, 2, 3, 4 and 6 (*cf.* Section 1.3.3.1 for a discussion of this basic result). The axis of an n-fold rotoreflection, *i.e.* an n-fold rotation followed or preceded by a reflection through a plane perpendicular to the rotation axis (such that neither the rotation nor the reflection is in general a symmetry operation) is designated by S_n, see Fig. 1.4.1.1(b) for S_4.

The following types of point groups exist:

(1) cyclic groups

(a) of rotations (C):

$$C_1,\ C_2,\ C_3,\ C_4,\ C_6;$$

(b) of rotoreflections (S, for the names in parentheses see later):

$$S_1\ (=C_{1h}=C_s),\ S_2\ (=C_i),\ S_3\ (=C_{3h}),\ S_4,\ S_6\ (=C_{3i}).$$

(2) In dihedral groups D_n an n-fold (vertical) rotation axis is accompanied by n symmetry-equivalent horizontal twofold rotation axes. The symbols are D_2 [in older literature, as in *IT* (1952), one also finds V instead of D_2, taken from the *Vierergruppe* of Klein (1884)], $D_3,\ D_4,\ D_6$; D_3 is visualized in Fig. 1.4.1.1(c).

(3) Other crystallographic point groups can be constructed by a C_n rotation axis or a D_n combination of rotation axes with a horizontal symmetry plane, leading to symbols C_{nh} or D_{nh}:

$$C_{2h}, C_{3h}, C_{4h}, C_{6h}, D_{2h}, D_{3h}, D_{4h}, D_{6h}.$$

The point groups C_{4h} and D_{6h} are represented by Figs. 1.4.1.1(d) and 1.4.1.1(e).

(4) Vertical rotation axes C_n can be combined with a vertical reflection plane, leading to n symmetry-equivalent vertical reflection planes (denoted v) which all contain the rotation axis:

$$C_{2v},\ C_{3v},\ C_{4v},\ C_{6v}$$

with Fig. 1.4.1.1(f) for C_{3v}.

(5) Combinations D_n of rotation axes may be combined with vertical reflection planes which bisect the angles between the horizontal twofold axes, such that the vertical planes (designated by the index d for 'diagonal') alternate with the horizontal twofold axes:

$$D_{2d} \text{ with } n=2 \text{ or } D_{3d} \text{ with } n=3;$$

see Fig. 1.4.1.1(g) for D_{3d}. In both point groups rotoreflections S_{2n}, *i.e.* S_4 or S_6, occur. Note that the classification of crystal classes into crystal systems follows the order of rotoinversions $\overline{N}$, not that of rotoreflections S_n (*cf.* Section 1.2.1 for the definition of rotoinversions). Therefore, D_{2d} is tetragonal ($S_4 \sim \overline{4}$) and D_{3d} is trigonal because of $S_6^5 = \overline{3}$). Analogously, C_{3h} and D_{3h} are hexagonal because they contain $S_3 \sim \overline{6}$. The point groups D_{4d} and D_{6d} are not crystallographic as they contain noncrystallographic eightfold or 12-fold rotoreflections S_8 or S_{12}.

(6) In all these groups the directions of the vectors $\pm$**c** are not equivalent to any other directions. There are, however, also cubic point groups and thus cubic space groups in which the basis vector **c** is symmetry-equivalent to both basis vectors **a** and **b**. T, T_h and T_d can be derived from the rotation group T of the tetrahedron, see Fig. 1.4.1.1(h). O and O_h can be derived from the rotation group O of the octahedron. The indices h and d have the same meaning as before.

(7) Some of these symbols are no longer used but are replaced by more visual ones. S_1 describes a reflection through a horizontal plane, it is replaced now by C_{1h} or by C_s; S_2 describes an inversion in a centre, it is replaced by C_i. The symbol S_3 describes the same arrangement as C_{3h} and is thus not used. S_6 contains an inversion centre combined with a threefold rotation axis and is replaced by C_{3i}.

The description of crystal classes using Schoenflies symbols is intuitive and much more graphic than that by Hermann–Mauguin symbols. It is useful for morphological studies investigating the symmetry of the ideal shape of crystals. Schoenflies symbols of crystal classes are also still used traditionally by physicists and chemists, in particular in spectroscopy and quantum chemistry.

1.4.1.3.2. Schoenflies symbols of the space groups

Different space groups of the same crystal class are distinguished by their superscript index, for example C_1^1; $D_{2h}^1, D_{2h}^2, \ldots, D_{2h}^{28}$ or $O_h^1, \ldots, O_h^{10}$.

Schoenflies symbols display the space-group symmetry only partly. Therefore, they are nowadays rarely used for the description of the symmetry of crystal structures. In comparison with the Schoenflies symbols, the Hermann–Mauguin symbols are more indicative of the space-group symmetry and that of the crystal structures.

1.4.1.4. Hermann–Mauguin symbols of the space groups

1.4.1.4.1. Introduction

The Hermann–Mauguin symbols, abbreviated as HM symbols in the following sections, were proposed by Hermann (1928, 1931) and Mauguin (1931), and introduced to the *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) according to the decision of the corresponding Programme Committee (Ewald, 1930). There are different kinds of HM symbols of a space group. One distinguishes *short HM symbols*, *full HM symbols* and *extended HM symbols*. The *full HM symbols* will be the basis of this description. They form the most transparent kind of HM symbols and their use will minimize confusion, especially for those who are new to crystallography.

As the name suggests, the *short HM symbols* are mostly shortened versions of the full HM symbols: some symmetry information of the full HM symbols is omitted such that these symbols are more convenient in daily use. The full HM symbol can be reconstructed from the short symbol. In the *extended HM symbols* the symmetry of the space group is listed in a more complete fashion (*cf.* Section 1.5.4). They are rarely used in crystallographic practice.

In the next section general features of the HM symbols will be discussed. Thereafter, the HM symbols for each crystal system will be presented in a separate section, because the appearance of

the HM symbols depends strongly on the crystal system to which the space group belongs.

1.4.1.4.2. General aspects

The Hermann–Mauguin symbol for a space group consists of a sequence of letters and numbers, here called the *constituents of the HM symbol*. The first constituent is always a symbol for the conventional cell of the translation lattice of the space group (*cf.* Section 1.3.2.1 for the definition of the translation lattice); the following constituents, namely rotations, screw rotations, rotoinversions, reflections and glide reflections, are marked by conventional symbols, *cf.* Table 2.1.2.1.[1] Together with the generating translations of the lattice, the set of these symmetry operations forms a *set of generating symmetry operations* of the space group. The space group can thus be generated from its HM symbol.

The symmetry operations of the constituents are referred to the lattice basis that is used conventionally for the crystal system of the space group. The kind of symmetry operation can be read from its symbol; the orientation of its geometric element, *cf.* de Wolff *et al.* (1989, 1992), *i.e.* its invariant axis or plane normal, can be concluded from the position of the corresponding constituent in the HM symbol, as the examples in the following sections will show. The origin is not specified. It is chosen by the user, who selects it in such a way that the matrices of the symmetry operations appear in the most convenient form. This is often, but not necessarily, the conventional origin chosen in the space-group tables of this volume. The choice of a different origin may make other tasks, *e.g.* the derivation of the space group from its generators, particularly easy and transparent.

The first constituent (the lattice symbol) characterizes the lattice of the space group referred to the conventional coordinate system. (Each lattice can be referred to a lattice basis, also called a *primitive basis*: the lattice vectors have only integer coefficients and the lattice is called a *primitive lattice*.) Lattice vectors with non-integer coefficients can occur if the lattice is referred to a non-primitive basis. In this way similarities and relations between different space-group types are emphasized.

The lattice symbol of a primitive basis consists of an upper-case letter *P* (**p**rimitive). Lattices with conventional non-primitive bases are called *centred lattices*, *cf.* Section 1.3.2.4 and Table 2.1.1.2. For these other letters are used: if the **ab** plane of the unit cell is centred with a lattice vector $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, the letter is *C*; for **ca** centring [($\frac{1}{2}(\mathbf{c}+\mathbf{a})$ as additional *centring vector*] the letter is *B*, and *A* is the letter for centring the **bc** plane of the unit cell by $\frac{1}{2}(\mathbf{b}+\mathbf{c})$. The letter is *F* for centring all side faces of the cell with centring vectors $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}(\mathbf{c}+\mathbf{a})$ and $\frac{1}{2}(\mathbf{b}+\mathbf{c})$. It is *I* (German: ***i**nnenzentriert*) for body centring by the vector $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ and *R* for the rhombohedral centring of the hexagonal cell by the vectors $\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c})$ and $\frac{1}{3}(\mathbf{a}+2\mathbf{b}+2\mathbf{c})$. In 1985, the letter *S* was introduced as a setting-independent 'centring symbol' for monoclinic and orthorhombic Bravais lattices (*cf.* de Woff *et al.*, 1985).

To describe the structure of the HM symbols the introduction of the term *symmetry direction* is useful.

Definition

A direction is called a *symmetry direction* of a crystal structure if it is parallel to an axis of rotation, screw rotation or rotoinversion or if it is parallel to the normal of a reflection or glide-reflection plane. A symmetry direction is thus the direction of the geometric element of a symmetry operation when the normal of a symmetry plane is used for the description of its orientation.

The corresponding symmetry operations [the *element set* of de Wolff *et al.* (1989 & 1992)] specify the type of the symmetry direction. The symmetry direction is always a lattice direction of the space group; the shortest lattice vector in the symmetry direction will be called **q**.

If **q** represents both a rotation or screw rotation and a reflection or glide reflection, then their symbols are connected in the HM symbol by a slash '/', *e.g.* 2/*m* or $4_1/a$ *etc*.

The symmetry directions of a space group form *sets of equivalent symmetry directions* under the symmetry of the space group. For example, in a cubic space group the **a**, **b** and **c** axes are equivalent and form the set of six directions ⟨100⟩: [100], [$\bar{1}$00], [010] *etc.* Another set of equivalent directions is formed by the eight space diagonals ⟨111⟩: [111], [1$\bar{1}\bar{1}$], ... If there are twofold rotations around the twelve face diagonals ⟨110⟩, as in the space group of the crystal structure of NaCl, ⟨110⟩ forms a third set of 12 symmetry directions.[2]

Instead of listing the symmetry operations (element set) for each symmetry direction of a set of symmetry directions, it is sufficient to choose one *representative direction of the set*. In the HM symbol, generators for the element set of each representative direction are listed.

It can be shown that there are zero (triclinic space groups), one (monoclinic), up to two (trigonal and rhombohedral) or up to three (most other space groups) sets of symmetry directions in each space group and thus zero, one, two or three representative symmetry directions.

The non-translation generators of a symmetry direction may include only one kind of symmetry operation, *e.g.* for twofold rotations 2 in space group *P*121, but they may also include several symmetry operations, *e.g.* 2, 2_1, *m* and *a* in space group *C*12/*m*1. To search for such directions it is helpful simply to look at the space-group diagrams to find out whether more than one kind of symmetry operation belongs to the generators of a symmetry direction. In general, only the simplest symbols are listed (*simplest-operation rule*): if we use '>' to mean '*has priority*', then pure rotations > screw rotations; pure rotations > rotoinversions; reflection $m > a, b, c > n$.[3] The space group mentioned above is conventionally called *C*12/*m*1 and not $C12_1/m1$ or $C12/a1$ or $C12_1/a1$.

The position of a plane is fixed by one parameter if its orientation is known. On the other hand, fixing an axis of known direction needs two parameters. Glide components also show two-dimensional variability, whereas there is only one parameter

[1] According to the recommendations of the International Union of Crystallography Ad Hoc Committee on the Nomenclature of Symmetry (de Wolff *et al.*, 1992), the characters appearing after the lattice letter in the HM symbol of a space group should represent symmetry elements, which is reflected, for example, in the introduction of the '*e*-glide' notation in the HM space-group symbols. To avoid misunderstandings, it is worth noting that in the following discussion of the HM symbolism, the author preferred to keep strictly to the original idea according to which the characters of the HM symbols were meant to represent (generating) symmetry operations of the space group, and not symmetry elements.

[2] The numbers listed are those for bipolar directions, for which direction and opposite direction are equivalent. For the corresponding polar directions in cubic space groups only the four equivalent polar directions ⟨111⟩ or ⟨1$\bar{1}\bar{1}$⟩ of the tetrahedron occur.

[3] The 'symmetry-element' interpretation of the constituents of the HM symbols (*cf.* footnote 1[1]) results in the following modification of the 'simplest-operation' rule [known as the 'priority rule', *cf.* Section 4.1.2.3 of *International Tables for Crystallography*, Volume A (2002) (referred to as *IT* A5)]: When more than one kind of symmetry element exists in a given direction, the choice of the corresponding symbols in the space-group symbol is made in order of descending priority $m > e > a, b, c > n$, and rotation axes before screw axes.

of a screw component. Therefore, reflections and glide reflections can better express the geometric relations between the symmetry operations than can rotations and screw rotations; reflections and glide reflections are more important for HM symbols than are rotations and screw rotations. The latter are frequently omitted to form short HM symbols from the full ones.

The second part of the *full HM symbol* of a space group consists of one position for each of up to three representative symmetry directions. To each position belong the generating symmetry operations of their representative symmetry direction. The position is thus occupied either by a rotation, screw rotation or rotoinversion and/or by a reflection or glide reflection.

The representative symmetry directions are different in the different crystal systems. For example, the directions of the basis vectors **a**, **b** and **c** are symmetry independent in orthorhombic crystals and are thus all representative, whereas **a** and **b** are symmetry equivalent and thus dependent in tetragonal crystals. All three directions are symmetry equivalent in cubic crystals; they belong to the same set and are represented by one of the directions. Therefore, the symmetry directions and their sequence in the HM symbols depend on the crystal system to which the crystal and thus its space group belongs.

Table 1.4.1.1
The structure of the Hermann–Mauguin symbols for the space groups

The positions of the representative symmetry directions for the different crystal systems are given. The description of the non-translational part of the HM symbol is always preceded by the lattice symbol, which in conventional settings is *P*, *A*, *B*, *C*, *F*, *I* or *R*. For monoclinic **b** setting and monoclinic **c** setting, *cf.* Section 1.4.1.4.4; the primitive hexagonal lattice is called *H* in this table.

Crystal system	First position	Second position	Third position
Triclinic (anorthic)	1 or $\bar{1}$	—	—
Monoclinic **b** setting Monoclinic **c** setting	1 1	**b** 1	1 **c**
Orthorhombic	**a**	**b**	**c**
Tetragonal	**c**	**a**	$\mathbf{a}-\mathbf{b}$
Trigonal *H* lattice	**c** **c**	**a** or 1	1 $\mathbf{a}-\mathbf{b}$
Trigonal, *R* lattice, hexagonal coordinates Trigonal, *R* lattice, rhombohedral coordinates	$\mathbf{c}_H$ $\mathbf{a}_R+\mathbf{b}_R+\mathbf{c}_R$	$\mathbf{a}_H$ or $\mathbf{a}_R-\mathbf{b}_R$	— —
Hexagonal	**c**	**a**	$\mathbf{a}-\mathbf{b}$
Cubic	**c**	$\mathbf{a}+\mathbf{b}+\mathbf{c}$	$\mathbf{a}-\mathbf{b}$

Table 1.4.1.1 gives the positions of the representative lattice-symmetry directions in the HM symbols for the different crystal systems.

Examples of full HM symbols are (from triclinic to cubic) $P\bar{1}$, $P12/c1$, $A112/m$, $F2/d2/d2/d$, $I4_1/a$, $P4/m2_1/n2/c$, $P\bar{3}$, $P3m1$, $P3_112$, $R\bar{3}2/c$, $P6_3/m$, $P6_122$ and $F4_132$.

There are crystal systems, for example tetragonal, for which the high-symmetry space groups display symmetry in all symmetry directions whereas lower-symmetry space groups display symmetry in only some of them. In such cases, the symmetry of the 'empty' symmetry direction is denoted by the constituent 1 or it is simply omitted. For example, instead of three symmetry directions in $P4mm$, there is only one in $I4_1/a11$, for which the HM symbol is usually written $I4_1/a$. However, in some trigonal space groups the designation of a symmetry direction by '1' ($P3_112$) is necessary to maintain the uniqueness of the HM symbols.[4]

The HM symbols can not only describe the space groups in their conventional settings but they can also indicate the setting of the space group relative to the conventional coordinate system mentioned in Section 1.4.1.3.1. For example, the orthorhombic space group $P2/m2/n2_1/a$ may appear as $P2/n2/m2_1/b$ or $P2/n2_1/c2/m$ or $P2_1/c2/n2/m$ or $P2_1/b2/m2/n$ or $P2/m2_1/a2/n$ depending on its orientation relative to the conventional coordinate basis. On the one hand this is an advantage, because the HM symbols include some indication of the orientation of the space group and form a more powerful tool than being just a space-group nomenclature. On the other hand, it is sometimes not easy to recognize the space-group type that is described by an unconventional HM symbol. In Section 1.4.1.4.5 an example is provided which deals with this problem.

[4] In the original HM symbols the constituent '1' was avoided by the use of different centred cells.

The full HM symbols describe the symmetry of a space group in a transparent way, but they are redundant. They can be shortened to the *short HM symbols* such that the set of generators is reduced to a necessary set. Examples will be displayed for the different crystal systems. The *conventional short HM symbols* still provide a unique description and enable the generation of the space group. For the monoclinic space groups with their many conventional settings they are not variable and are taken as standard for their space-group types. Monoclinic short HM symbols may look quite different from the full HM symbol, *e.g.* Cc instead of $A1n1$ or $I1a1$ or $B11n$ or $I11b$.

The *extended HM symbols* display the additional symmetry that is often generated by lattice centrings. The full HM symbol denotes only the simplest symmetry operations for each symmetry direction, by the 'simplest symmetry operation' rule; the other operations can be found in the extended symbols, which are treated in detail in Section 1.5.4 and are listed in Tables 1.5.4.3 (plane groups) and 1.5.4.4 (space groups).

From the HM symbol of the space group, the full or short *HM symbol for a crystal class* of a space group is obtained easily: one omits the lattice symbol, cancels all screw components such that only the symbol for the rotation is left and replaces any letter for a glide reflection by the letter *m* for a reflection. Examples are $P2_1/b2_1/a2/m \rightarrow 2/m2/m2/m$ and $I4_1/a11 \rightarrow 4/m$.

If one is not yet familiar with the HM symbols, it is recommended to start with the orthorhombic space groups in Section 1.4.1.4.5. In the orthorhombic crystal system all crystal classes have the same number of symmetry directions and the HM symbols are particularly transparent. Therefore, the orthorhombic HM symbols are explained in more detail than those of the other crystal systems.

The following discussion treats mainly the HM symbols of space groups in conventional settings; for non-conventional descriptions of space groups the reader is referred to Chapter 1.5.

1.4.1.4.3. Triclinic space groups

There is no symmetry direction in a triclinic space group. Therefore, the basis vectors of a triclinic space group can always be chosen to span a primitive cell and the HM symbols are $P1$ (without inversions) and $P\bar{1}$ (with inversions). The HM symbol

$P\bar{1}$ is the only one which displays the inversion $\bar{1}$ explicitly. Sometimes non-conventional centred lattice descriptions may be used, especially when comparing crystal structures.

1.4.1.4.4. Monoclinic space groups

Monoclinic space groups have exactly one symmetry direction, often called *the monoclinic axis*. The *b* axis is the symmetry direction of the (most frequently used) conventional setting, called the *b*-axis setting. Another conventional setting has **c** as its symmetry direction (*c*-axis setting). In earlier literature, the unique-axis *c* setting was called the first setting and the unique-axis *b* setting the second setting (*cf.* Section 2.1.3.15). In addition to the primitive lattice *P* there is a centred lattice which is taken as *C* in the *b*-axis setting, *A* in the *c*-axis setting. The (possible) glide reflections are *c* (or *a*). In this volume, more settings are described, *cf.* Sections 1.5.4 and 2.1.3.15 and the space-group tables of Chapter 2.3.

The full HM symbol consists of the lattice symbol and three possible positions for the symmetry directions. The symmetry in the **a** direction is described first, followed by the symmetry in the **b** direction and last in the **c** direction. The two positions of the HM symbol that are not occupied by the monoclinic symmetry direction are marked by 1. The symbol is thus similar to the orthorhombic HM symbol and the monoclinic axis is clearly visible. *P*1*m*1 or *P*11*m* may designate the same space group but in different settings. *Pm*11 is a possible but not conventional setting.

The short HM symbols of the monoclinic space groups are independent of the setting of the space group. They form the *monoclinic standard symbols* and are not variable: *P*2, $P2_1$, *C*2, *Pm*, *Pc*, *Cm*, *Cc*, *P*2/*m*, $P2_1/m$, *C*2/*m*, *P*2/*c*, $P2_1/c$ and *C*2/*c*. Altogether there are 13 monoclinic space-group types.

There are several reasons for the many conventional settings.

(1) As only one of the three coordinate axes is fixed by symmetry, there are two conventions related to the possible permutations of the other axes.
(2) The sequence of the three coordinate axes may be chosen because of the lengths of the basis vectors, *i.e.* not because of symmetry.
(3) If two different crystal structures have related symmetries, one being a subgroup of the other, then it is often convenient to choose a non-conventional setting for one of the structures to make their structural relations transparent. Such similarity happens in particular in substances that are related by a non-destructive phase transition. Monoclinic space groups are particularly flexible in their settings.

1.4.1.4.5. Orthorhombic space groups

To the orthorhombic crystal system belong the crystal classes 222, *mm*2 and 2/*m* 2/*m* 2/*m* with the Bravais types of lattices *P*, *C*, *A*, *F* and *I*. Four space groups with a *P* lattice belong to the crystal class 222, ten to *mm*2 and 16 to 2/*m* 2/*m* 2/*m*. Each of the basis vectors marks a symmetry direction; the lattice symbol is followed by characters representing the symmetry operations with respect to the symmetry directions along **a**, **b** and **c**.

We start with the full HM symbols. For a space group of crystal class 222 with a *P* lattice the HM symbol is thus '$PR_1R_2R_3$', where R_1, R_2, $R_3 = 2$ or 2_1. Conventionally one chooses a setting with the symbols *P*222, $P222_1$, $P2_12_12$ and $P2_12_12_1$.

For the generation of the space groups of this crystal class only two non-translational generators are necessary, say R_1 and R_2. However, it is not possible to indicate in the HM symbol whether the axes R_1 and R_2 intersect or not. This is decided by the third (screw) rotation R_3: if $R_3 = R_1R_2 = 2$, the axes R_1 and R_2 intersect, if $R_3 = 2_1$, they do not. For this reason, R_3 is sometimes called an *indicator*. However, any two of the three rotations or screw rotations can be taken as the generators and the third one is then the indicator. Mathematically each element of a generating set is a generator independent of its possible redundancy.

In the space groups of crystal class *mm*2 the two reflections or glide reflections are the generators, the twofold rotation or screw rotation is generated by composition of the (glide) reflections. The position of the rotation axis relative to the intersection line of the two planes as well as its screw component are determined uniquely by the glide components of the reflections or glide reflections.

The rotation or screw rotation in the HM symbols of space groups of the crystal class *mm*2 could be omitted, and were omitted in older HM symbols. Nowadays they are included to make the orthorhombic HM symbols more homogeneous. Conventional symbols are, among others, *Pmm*2, $Pmc2_1$, *Pba*2 and $Pca2_1$.

The 16 space groups with a *P* lattice in crystal class 2/*m* 2/*m* 2/*m* are similarly obtained by starting with the letter *P* and continuing with the point-group symbol, modified by the possible replacements 2_1 for 2 and *a*, *b*, *c* or *n* for *m*. The conventional symbols are, among others, *P*2/*m* 2/*m* 2/*m*, $P2_1/m\,2/m\,2/a$, $P2/m\,2/n\,2_1/a$, $P2_1/b\,2_1/a\,2/m$ or $P2_1/n\,2_1/m\,2_1/a$. The symbols $P2/m\,2/n\,2_1/a$ and $P2_1/n\,2_1/m\,2_1/a$ designate different space-group types, as is easily seen by looking at the screw rotations: $P2/m\,2/n\,2_1/a$ has screw axes in the direction of **c** only, $P2_1/n\,2_1/m\,2_1/a$ has screw axes in all three symmetry directions.

If the lattice is centred, the constituents in the same symmetry direction are not unique. In this case, according to the 'simplest symmetry operation' rule, in general the simplest operation is chosen, *cf.* Section 1.5.4.

Examples

In the HM symbol $C2/m\,2/c\,2_1/m$ there are in addition 2_1 screw rotations in the first two symmetry directions; additional glide reflections *b* occur in the first, and *n* in the second and third symmetry directions.

In $I2/b\,2/a\,2/m$, all rotations 2 are accompanied by screw rotations 2_1; *b* and *a* are accompanied by *c* and *m* is accompanied by *n*. The symmetry operations that are not listed in the full HM symbol can be derived by composition of the listed operations with a centring translation, *cf.* Section 1.4.2.4.

There are two exceptions to the 'simplest symmetry operation' rule. If the *I* centring is added to the *P* space groups of the crystal class 222, one obtains two different space groups with an *I* lattice, each has 2 and 2_1 operations in each of the symmetry directions. One space group is derived by adding the *I* centring to the space group *P*222, the other is obtained by adding the *I* centring to a space group $P2_12_12_1$. In the first case the twofold axes intersect, in the second they do not. According to the rules both should get the HM symbol *I*222, but only the space group generated from *P*222 is named *I*222, whereas the space group generated from $P2_12_12_1$ is called $I2_12_12_1$. The second exception occurs among the cubic space groups and is due to similar reasons, *cf.* Section 1.4.1.4.8.

The *short HM symbols* for the space groups of the crystal classes 222 and *mm*2 are the same as the full HM symbols. In the short HM symbols for the space groups of the crystal class 2/*m* 2/*m* 2/*m* the symbols for the (screw) rotations are omitted, resulting in the short symbols *Pmmm*, *Pmma*, *Pmna*, *Pbam*, *Pnma*, *Cmcm* and *Ibam* for the space groups mentioned above.

These are HM symbols of space groups in conventional settings. It is less easy to find the conventional HM symbol and the space-group type from an unconventional short HM symbol. This may be seen from the following example:

Question: Given the short HM symbols *Pman*, *Pmbn* and *Pmcn*, what are the conventional descriptions of their space-group types, and are they identical or different?

Answer: A glance at the HM symbols shows that the second symbol does not describe any space-group type at all. The second symmetry direction is **b**; the glide plane is perpendicular to it and the glide component may be $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{c}$ or $\frac{1}{2}(\mathbf{c}+\mathbf{a})$, but not $\frac{1}{2}\mathbf{b}$.

In this case it is convenient to define the intersection of the three (glide) reflection planes as the site of the origin. Then all translation components of the generators are zero except the glide components.

(1) *Pman*. If one names the three (glide) reflections according to the directions of their normals by m_{100}, a_{010} and n_{001}, then $a_{010}n_{001} = 2_{100}$, $m_{100}a_{010} = 2_{001}$, while the composition $n_{001}m_{100}$ results in a 2_1 screw rotation along [010].

Clearly, the unconventional full HM symbol is $P\,2/m\,2_1/a\,2/n$. The procedure for obtaining from this symbol the conventional HM symbol $P\,2/m\,2/n\,2_1/a$ (or short symbol *Pmna*) with the origin at the inversion centre is described in Chapter 1.5.

(2) *Pmcn*. Using a nomenclature similar to that of (1), one obtains 2_1 screw axes along [100], [010] and [001] by the compositons $c_{010}n_{001}$, $n_{001}m_{100}$ and $m_{100}c_{010}$, respectively. Thus the unconventional full HM symbol is $P\,2_1/m\,2_1/c\,2_1/n$. Again, the procedure of Chapter 1.5 results in the full HM symbol $P\,2_1/n\,2_1/m\,2_1/a$ or the short symbol *Pnma*. The full HM symbols show that the two space-group types are different.

1.4.1.4.6. Tetragonal space groups

There are seven tetragonal crystal classes. The lattice may be *P* or *I*. The space groups of the three crystal classes 4, $\overline{4}$ and 4/*m* have only one symmetry direction, [001]. The other four classes, 422, 4*mm*, $\overline{4}2m$ and $4/m\,2/m\,2/m$ display three symmetry directions which are listed in the sequence [001], [100] and $[1\bar{1}0]$.[5]

1.4.1.4.6.1. Tetragonal space groups with one symmetry direction

In the space groups of the crystal class 4, rotation or screw rotation axes run in direction [001]; in the space groups of crystal class $\overline{4}$ these are rotoinversion axes $\overline{4}$; and in crystal class 4/*m* both occur. The rotation 4 of the point group may be replaced by screw rotations 4_1, 4_2 or 4_3 in the space groups with a *P* lattice. If the lattice is *I*-centred, 4 and 4_2 or 4_1 and 4_3 occur simultaneously, together with $\overline{4}$ rotoinversions.

In the space groups of crystal class 4/*m* with a *P* lattice, the rotations 4 can be replaced by the screw rotations 4_2 and the reflection *m* by the glide reflection *n* such that four space-group types with a *P* lattice exist: *P*4/*m*, $P4_2/m$, *P*4/*n* and $P4_2/n$. Two more are based on an *I* lattice: *I*4/*m* and $I4_1/a$. In all these six space groups the short HM symbols and full HM symbols are the same.

[5] One usually chooses $[1\bar{1}0]$ as the representative direction and not the equivalent direction [110], in analogy to the cases of trigonal and hexagonal space groups where $[1\bar{1}0]$ is the representative of the set of tertiary symmetry directions, while $[\bar{1}10]$ (or [110]) belongs to the set of secondary symmetry directions, *cf.* Table 2.1.3.1.

1.4.1.4.6.2. Tetragonal space groups with three symmetry directions

There are four crystal classes with three symmetry directions each. In the corresponding space-group symbols the constituents 2, 4 and *m* may be replaced by 2_1, 4_k with $k = 1$, 2 or 3, and *a*, *b*, *c*, *n* or *d*, respectively. The constituent $\overline{4}$ persists. Full HM symbols of space groups are, among others, $P4_22_12$, $P4_2bc$, $P\overline{4}2c$ and $I\,4_1/a\,2/c\,2/d$.

The full and short HM symbols agree for the space groups that belong to the crystal classes 422, 4*mm* and $\overline{4}2m$. Only for the space groups of $4/m\,2/m\,2/m$ have the short HM symbols lost their twofold rotations or screw rotations leading, *e.g.*, to the symbol $I4_1/acd$ instead of $I\,4_1/a\,2/c\,2/d$.

Example

In *P*4*mm*, to the primary symmetry direction [001] belong the rotation 4 and its powers, to the secondary symmetry direction [100] belongs the reflection m_{100}. However, in the tertiary symmetry direction $[1\bar{1}0]$, there occur reflections *m* and glide reflections *g* with a glide vector $\frac{1}{2}(\mathbf{a}+\mathbf{b})$. Such glide reflections are not listed in the 'symmetry operations' blocks of the space-group tables if they are composed of a representing *general position* and an integer translation, as happens here (*cf.* Section 1.4.2.4 and Section 1.5.4 for a detailed discussion of the additional symmetry operations generated by combinations with integer translations). Glide reflections may have complicated glide vectors. If these do not fit the labels *a*, *b*, *c*, *n* or *d*, they are frequently called *g*.

1.4.1.4.7. Trigonal, hexagonal and rhombohedral space groups

Hexagonal and trigonal space groups are referred to a hexagonal coordinate system *P* with basis vector $\mathbf{c} \perp (\mathbf{a}, \mathbf{b})$. The basis vectors **a** and **b** span a hexagonal net and form an angle of 120°. The sequence of the representatives of the (up to three) symmetry directions is [001], [100] and $[1\bar{1}0]$. Usually, the seven trigonal space groups of the rhombohedral lattice system (or *rhombohedral space groups* for short) are described either with respect to a hexagonal coordinate system (triple hexagonal cell) or to a rhombohedral coordinate system (primitive rhombohedral cell).

1.4.1.4.7.1. Trigonal space groups

Trigonal space groups are characterized by threefold rotation or screw rotation or rotoinversion axes in [001]. There may be in addition 2 and 2_1 axes in [100] or $[1\bar{1}0]$, but only in one of these two directions. The same holds for reflections *m* or glide reflections *c*. The different possibilities are:

(1) There are only threefold axes 3 or 3_1 or 3_2 or $\overline{3}$. The short and the full HM symbols are *P*3, $P3_1$, $P3_2$, $P\overline{3}$.

(2) There are in addition horizontal twofold axes. Their direction is either [100] or $[1\bar{1}0]$. The corresponding position of the HM symbol is marked by 2, the other (empty) position is marked by 1: *P*321, *P*312, $P3_121$, $P3_112$ *etc. Note*: *P*321 and *P*312 denote *different* space-group types.

(3) In addition to the threefold axes, there are reflection planes or glide planes with their representative normals in the horizontal directions [100] or $[1\bar{1}0]$. The corresponding position of the HM symbol is marked by *m* or *c*, the empty position is marked by 1: *P*3*m*1 or *P*31*m etc.*

(4) The main axis in [001] is $\overline{3}$. Because $\overline{3}$ contains an inversion, the second or third position in the full HM symbol is marked by 2/*m* or 2/*c*, which leads to the HM symbols $P\,\overline{3}\,2/m\,1$ or

$P\bar{3}\,1\,2/m$ *etc.* In the short HM symbol the '2/' is not kept: $P\bar{3}m1$ or $P\bar{3}1m$ *etc.*

1.4.1.4.7.2. Hexagonal space groups

Hexagonal space groups have either one or three representative symmetry directions. The space groups of crystal classes 6, $\bar{6}$ and $6/m$ have [001] as their single symmetry direction for the axis 6 or 6_k for $k = 1, \ldots, 5$ or $\bar{6}$, and for the plane m with its normal along [001]. The short and full HM symbols are the same. Examples are $P6$, $P6_4$, $P\bar{6}$ and $P6_3/m$.

Space groups of crystal classes 622, $6mm$, $\bar{6}2m$ and $6/m\,2/m\,2/m$ have the representative symmetry directions [001], [100] and $[1\bar{1}0]$. As opposed to the trigonal HM symbols, in the hexagonal HM symbols no symmetry direction is 'empty' and occupied by '1'.

In space groups of the crystal classes 622, $6mm$ and $\bar{6}2m$ the short and full HM symbols are the same; in $6/m\,2/m\,2/m$ the short symbols are deprived of the parts '2/' of the full symbols. The full HM symbol $P\,6_3/m\,2/m\,2/c$ is shortened to the short HM symbol $P6_3/mmc$, the full HM symbol $P\,6_3/m\,2/c\,2/m$ is shortened to $P6_3/mcm$. The two denote different space-group types.

1.4.1.4.7.3. Rhombohedral space groups

The rhombohedral lattice may be understood as an R-centred hexagonal lattice and then referred to the hexagonal basis. It has two kinds of symmetry directions, which coincide with the primary and secondary symmetry directions of the hexagonal lattice (owing to the R centrings, no symmetry operation along the tertiary symmetry direction of the hexagonal lattice is compatible with the rhombohedral lattice). On the other hand, the rhombohedral lattice may be referred to a (primitive) rhombohedral coordinate system with the lattice parameters $a = b = c$ and $\alpha = \beta = \gamma$. The HM symbol of a rhombohedral space group starts with R, its representative symmetry directions are $[001]_{\rm hex}$ or $[111]_{\rm rhomb}$ and $[100]_{\rm hex}$ or $[1\bar{1}0]_{\rm rhomb}$. In this section the rhombohedral primitive cell is used. The rotations 3 and the rotoinversions $\bar{3}$ are accompanied by screw rotations 3_1 and 3_2. Rotations 2 about horizontal axes always alternate with 2_1 screw rotations and reflections m are accompanied by different glide reflections g with unconventional glide components. The additional operations mentioned are not listed in the full HM symbols.

The seven rhombohedral space groups belong to the five crystal classes 3, $\bar{3}$, 32, $3m$ and $\bar{3}2/m$. In $R3$ and $R\bar{3}$ only the first of the symmetry directions is occupied and listed in the full and short HM symbols. In the space groups of the other crystal classes the second symmetry direction $[1\bar{1}0]$ is occupied by '2' or 'm' or 'c' or '$2/m$' or '$2/c$', leading to the full HM symbols $R32$, $R3m$, $R3c$, $R\bar{3}2/m$ and $R\bar{3}2/c$. In the short HM symbols the '2/' parts of the last two symbols are skipped: $R\bar{3}m$ and $R\bar{3}c$.

1.4.1.4.8. Cubic space groups

There are five cubic crystal classes combined with the three types of lattices P, F and I in which the cubic space groups are classified. The two symmetry directions [100] and [111] are the representative directions in the space groups of the crystal classes 23 and $2/m\,\bar{3}$. A third representative symmetry direction, $[1\bar{1}0]$, is added for space groups of the crystal classes 432, $\bar{4}3m$ and $4/m\,\bar{3}\,2/m$.[6]

[6] Note: '3' or '$\bar{3}$' directly after the lattice symbol denotes a trigonal or rhombohedral space group; '3' or '$\bar{3}$' in the third position (second position after the lattice symbol) is characteristic for cubic space groups.

Table 1.4.1.2
The structure of the Hermann–Mauguin symbols for the plane groups

The positions of the representative symmetry directions for the crystal systems are given. The lattice symbol and the maximal order of rotations around a point are followed by two positions for symmetry directions.

Crystal system	Lattice(s)	First position	Second position	Third position
Oblique	p	1 or 2	—	—
Rectangular	p, c	1 or 2	**a**	**b**
Tetragonal	p	4	**a**	**a** − **b**
Hexagonal	p	3	**a**	1
			or	
		3	1	**a** − **b**
		6	**a**	**a** − **b**

In the full HM symbol the symmetry is described as usual. Examples are $P2_13$, $F\,2/d\,\bar{3}$, $P4_332$, $F\bar{4}3c$, $P\,4_2/m\,\bar{3}\,2/n$ and finally No. 230, $I\,4_1/a\,\bar{3}\,2/d$. The short HM symbols of the noncentrosymmetric space groups (those of crystal classes 23, 432 and $\bar{4}3m$) are the same as the full HM symbols. In the short HM symbols of centrosymmetric space groups of the crystal classes $2/m\,\bar{3}$ and $4/m\,\bar{3}\,2/m$ the rotations or screw rotations are omitted with the exception of the rotations 3 and rotoinversions $\bar{3}$ which represent the symmetry in direction [111]. Thus, in the examples listed above, $Fd\bar{3}$, $Pm\bar{3}n$ and $Ia\bar{3}d$ are the short HM symbols differing from the full HM symbols.

As in the orthorhombic space groups $I222$ and $I2_12_12_1$, there is the pair $I23$ and $I2_13$ in which the 'simplest symmetry operation' rule is violated. In both space groups twofold rotations and screw rotations around **a**, **b** and **c** occur simultaneously. In $I23$ the rotation axes intersect, in $I2_13$ they do not. The first space group can be generated by adding the I-centring to the space group $P23$, the second is obtained by adding the I-centring to the space group $P2_13$.

1.4.1.5. Hermann–Mauguin symbols of the plane groups

The principles of the HM symbols for space groups are retained in the HM symbols for plane groups (also known as *wallpaper groups*). The rotation axes along **c** of three dimensions are replaced by *rotation points* in the **ab** plane; the possible orders of rotations are the same as in three-dimensional space: 2, 3, 4 and 6. The lattice (sometimes called *net*) of a plane group is spanned by the two basis vectors **a** and **b**, and is designated by a lower-case letter. The choice of a lattice basis, *i.e.* of a minimal cell, leads to a primitive lattice p, in addition a c-centred lattice is conventionally used. The nets are listed in Table 3.1.2.1. The reflections and glide reflections through planes of the space groups are replaced by *reflections and glide reflections through lines*. Glide reflections are called g independent of the direction of the glide line. The arrangement of the constituents in the HM symbol is displayed in Table 1.4.1.2.

Short HM symbols are used only if there is at most one symmetry direction, *e.g.* $p411$ is replaced by $p4$ (no symmetry direction), $p1m1$ is replaced by pm (one symmetry direction) *etc.*

There are four crystal systems of plane groups, *cf.* Table 3.2.3.1. The analogue of the triclinic crystal system is called *oblique*, the analogues of the monoclinic and orthorhombic crystal systems are *rectangular*. Both have rotations of order 2 at most. The presence of reflection or glide reflection lines in the rectangular crystal system allows one to choose a rectangular basis with one basis vector perpendicular to a symmetry line and one basis

vector parallel to it. The *square* crystal system is analogous to the tetragonal crystal system for space groups by the occurrence of fourfold rotation points and a square net. Plane groups with threefold and sixfold rotation points are united in the *hexagonal* crystal system with a hexagonal net.

Plane groups occur as sections and projections of the space groups, *cf.* Section 1.4.5. In order to maintain the relations to the space groups, the symmetry directions of the symmetry lines are determined by their normals, not by the directions of the lines themselves. This is important because the normal of the line, not the direction of the line itself, determines the position in the HM symbol.

(1) In oblique plane groups there is no symmetry direction: HM symbols are $p1$ or $p2$.

(2) Rectangular plane groups may have no rotations and then only one symmetry direction: $p1m1 = pm$, $p1g1 = pg$ and $c1m1 = cm$. If there are twofold rotations, the HM symbol starts with $p2$ or $c2$, followed by the symmetry m or g first perpendicular to **a** and then perpendicular to **b**. The conventional HM symbol $p2mg$ describes a plane group with a reflection line running perpendicular to **a** (parallel to **b**) and a glide-reflection line running from the back to the front (perpendicular to **b** and thus parallel to **a**). There are four plane-group types: $p2mm$, $p2mg$, $p2gg$ and $c2mm$. The constituent '2' was sometimes omitted in older HM symbols.

(3) There is one square plane group with only rotations and no symmetry directions, the net is a square net: $p411 = p4$. The generating symmetry of symmetry directions perpendicular to **a** and **a** − **b** are listed in the second and third positions: $p4mm$ with reflection lines perpendicular to **a** and **b** and $p4gm$ with glide lines in the same directions. Reflection lines and glide lines perpendicular to **a** − **b** (and **a** + **b**) alternate.

(4) Five plane groups belong to the hexagonal crystal system. The trigonal and hexagonal plane groups $p311 = p3$ and $p611 = p6$ contain only rotations. In the other trigonal plane groups there is exactly one set of symmetry directions; its representative direction is either perpendicular to **a** ($p3m1$) or perpendicular to **a** − **b** ($p31m$).

The HM symbols $p3m1$ and $p31m$ may be easily confused, although they are different. Apart from the different orientations of their symmetry directions, in a plane group of type $p3m1$, all rotation points lie on reflection lines, but in $p31m$ not all of them do.

The hexagonal plane group $p6mm$ displays representative directions of mirror lines perpendicular to **a** *and* perpendicular to **a** − **b**.

1.4.1.6. Sequence of space-group types

The sequence of space-group entries in the space-group tables follows that introduced by Schoenflies (1891) and is thus established historically. Within each geometric crystal class, Schoenflies numbered the space-group types in an obscure way. As early as 1919, Niggli (1919) considered this Schoenflies sequence to be unsatisfactory and suggested that another sequence might be more appropriate. Fedorov (1891) used a different sequence in order to distinguish between symmorphic, hemisymmorphic and asymmorphic space groups (*cf.* Section 1.3.3.3 for a detailed discussion of symmorphic space groups).

The basis of the Schoenflies symbols and thus of the Schoenflies listing is the geometric crystal class. For the present space-group tables, a sequence might have been preferred in which, in addition, space-group types belonging to the same arithmetic crystal class were grouped together. It was decided, however, that the long-established sequence in the earlier editions of *International Tables* should not be changed.

In Table 1.4.1.3, those geometric crystal classes are listed in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class (*cf.* Section 1.3.4.4 for the definition and discussion of arithmetic crystal classes). The space

Table 1.4.1.3
List of geometric crystal classes in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class

Geometric crystal class	Space-group type		
	No.	Hermann–Mauguin symbol	Schoenflies symbol
$2/m$	10	$P2/m$	C_{2h}^1
	11	$P2_1/m$	C_{2h}^2
	13	$P2/c$	C_{2h}^4
	14	$P2_1/c$	C_{2h}^5
	12	$C2/m$	C_{2h}^3
	15	$C2/c$	C_{2h}^6
32	149	$P312$	D_3^1
	151	$P3_112$	D_3^3
	153	$P3_212$	D_3^5
	150	$P321$	D_3^2
	152	$P3_121$	D_3^4
	154	$P3_221$	D_3^6
	155	$R32$	D_3^7
$3m$	156	$P3m1$	C_{3v}^1
	158	$P3c1$	C_{3v}^3
	157	$P31m$	C_{3v}^2
	159	$P31c$	C_{3v}^4
	160	$R3m$	C_{3v}^5
	161	$R3c$	C_{3v}^6
23	195	$P23$	T^1
	198	$P2_13$	T^4
	196	$F23$	T^2
	197	$I23$	T^3
	199	$I2_13$	T^5
$m\bar{3}$	200	$Pm\bar{3}$	T_h^1
	201	$Pn\bar{3}$	T_h^2
	205	$Pa\bar{3}$	T_h^6
	202	$Fm\bar{3}$	T_h^3
	203	$Fd\bar{3}$	T_h^4
	204	$Im\bar{3}$	T_h^5
	206	$Ia\bar{3}$	T_h^7
432	207	$P432$	O^1
	208	$P4_232$	O^2
	213	$P4_132$	O^7
	212	$P4_332$	O^6
	209	$F432$	O^3
	210	$F4_132$	O^4
	211	$I432$	O^5
	214	$I4_132$	O^8
$\bar{4}3m$	215	$P\bar{4}3m$	T_d^1
	218	$P\bar{4}3n$	T_d^4
	216	$F\bar{4}3m$	T_d^2
	219	$F\bar{4}3c$	T_d^5
	217	$I\bar{4}3m$	T_d^3
	220	$I\bar{4}3d$	T_d^6

groups are rearranged in such a way that space groups of the same arithmetic crystal class are grouped together. The arithmetic crystal classes are separated by rules spanning the last three columns of the table and the geometric crystal classes are separated by rules spanning the full width of the table. In all cases not listed in Table 1.4.1.3, the Schoenflies sequence, as used in the space-group tables, does not break up arithmetic crystal classes. Nevertheless, some rearrangement would be desirable in other arithmetic crystal classes too. For example, the symmorphic space group should always be the first entry of each arithmetic crystal class.

1.4.2. Descriptions of space-group symmetry operations

By M. I. Aroyo, G. Chapuis, B. Souvignier and A. M. Glazer

One of the aims of the space-group tables of Chapter 2.3 is to represent the symmetry operations of each of the 17 plane groups and 230 space groups. The following sections offer a short description of the symbols of the symmetry operations, their listings and their graphical representations as found in the space-group tables of Chapter 2.3. For a detailed discussion of crystallographic symmetry operations and their matrix–column presentation ($\boldsymbol{W}$, $\boldsymbol{w}$) the reader is referred to Chapter 1.2.

1.4.2.1. Symbols for symmetry operations

Given the analytical description of the symmetry operations by matrix–column pairs ($\boldsymbol{W}$, $\boldsymbol{w}$), their geometric meaning can be determined following the procedure discussed in Section 1.2.2. The notation scheme of the symmetry operations applied in the space-group tables was designed by W. Fischer and E. Koch, and the following description of the symbols partly reproduces the explanations by the authors given in Section 11.1.2 of *IT* A5. Further explanations of the symbolism and examples are presented in Section 2.1.3.9.

The symbol of a symmetry operation indicates the type of the operation, its screw or glide component (if relevant) and the location of the corresponding geometric element (*cf.* Section 1.2.3 and Table 1.2.3.1 for a discussion of geometric elements). The symbols of the symmetry operations explained below are based on the Hermann–Mauguin symbols (*cf.* Section 1.4.1.4), modified and supplemented where necessary.

The symbol for the *identity* mapping is 1.

A *translation* is symbolized by the letter t followed by the components of the translation vector between parentheses. *Example*: $t(\frac{1}{2}, \frac{1}{2}, 0)$ represents a translation by a vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$, *i.e.* a C centring.

A *rotation* is symbolized by a number $n = 2$, 3, 4 or 6 (according to the rotation angle $360^\circ/n$) and a superscript + or −, which specifies the sense of rotation ($n > 2$). The symbol of rotation is followed by the location of the rotation axis. *Example*: 4^+ $0, y, 0$ indicates a rotation of 90° about the line $0, y, 0$ that brings point $0, 0, 1$ onto point $1, 0, 0$, *i.e.* a counter-clockwise rotation (or rotation in the mathematically *positive sense*) if viewed from point $0, 1, 0$ to point $0, 0, 0$.

A *screw rotation* is symbolized in the same way as a pure rotation, but with the screw part added between parentheses. *Example*: $3^-(0, 0, \frac{1}{3})$ $\frac{2}{3}, \frac{1}{3}, z$ indicates a clockwise rotation of 120° around the line $\frac{2}{3}, \frac{1}{3}, z$ (or rotation in the mathematically *negative sense*) if viewed from the point $\frac{2}{3}, \frac{1}{3}, 1$ towards $\frac{2}{3}, \frac{1}{3}, 0$, combined with a translation of $\frac{1}{3}\mathbf{c}$.

A *reflection* is symbolized by the letter m, followed by the location of the mirror plane.

A *glide reflection* in general is symbolized by the letter g, with the glide part given between parentheses, followed by the location of the glide plane. These specifications characterize every glide reflection uniquely. Exceptions are the traditional symbols a, b, c, n and d that are used instead of g. In the case of a glide plane a, b or c, the explicit statement of the glide vector is omitted if it is $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$ or $\frac{1}{2}\mathbf{c}$, respectively. *Examples*: a $x, y, \frac{1}{4}$ means a glide reflection with glide vector $\frac{1}{2}\mathbf{a}$ and through a plane $x, y, \frac{1}{4}$; $d(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ $x, x - \frac{1}{4}, z$ denotes a glide reflection with glide part $(\frac{1}{4}, \frac{1}{4}, \frac{3}{4})$ and the glide plane d at $x, x - \frac{1}{4}, z$.

An *inversion* is symbolized by $\bar{1}$ followed by the location of the inversion centre.

A *rotoinversion* is symbolized, in analogy with a rotation, by $\bar{3}$, $\bar{4}$ or $\bar{6}$ and the superscript + or −, again followed by the location of the (rotoinversion) axis. Note that angle and sense of rotation refer to the pure rotation and not to the combination of rotation and inversion. In addition, the location of the inversion point is given by the appropriate coordinate triplet after a semicolon. *Example*: $\bar{4}^+$ $0, \frac{1}{2}, z$; $0, \frac{1}{2}, \frac{1}{4}$ means a 90° rotoinversion with axis at $0, \frac{1}{2}, z$ and inversion point at $0, \frac{1}{2}, \frac{1}{4}$. The rotation is performed in the mathematically positive sense when viewed from $0, \frac{1}{2}, 1$ towards $0, \frac{1}{2}, 0$. Therefore, the rotoinversion maps point $0, 0, 0$ onto point $-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$.

The notation scheme is extensively applied in the symmetry-operations blocks of the space-group descriptions in the tables of Chapter 2.3. The numbering of the entries of the symmetry-operations block corresponds to that of the coordinate triplets of the general position, and in space groups with primitive cells the two lists contain the same number of entries. As an example consider the symmetry-operations block of the space group $P2_1/c$ shown in Fig. 1.4.2.1. The four entries correspond to the four coordinate triplets of the general-position block of the group and provide the geometric description of the symmetry operations chosen as

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$

Figure 1.4.2.1
General-position and symmetry-operations blocks for the space group $P2_1/c$, No. 14 (unique axis b, cell choice 1). The coordinate triplets of the general position, numbered from (1) to (4), correspond to the four coset representatives of the decomposition of $P2_1/c$ with respect to its translation subgroup, *cf.* Table 1.4.2.6. The entries of the symmetry-operations block numbered from (1) to (4) describe geometrically the symmetry operations represented by the four coordinate triplets of the general-position block.

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
16 e 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$

Symmetry operations

For $(0,0,0)+$ set			
(1) 1	(2) 2 $0,0,z$	(3) m $x,0,z$	(4) m $0,y,z$
For $(0,\frac{1}{2},\frac{1}{2})+$ set			
(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) c $x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
For $(\frac{1}{2},0,\frac{1}{2})+$ set			
(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(4) c $\frac{1}{4},y,z$
For $(\frac{1}{2},\frac{1}{2},0)+$ set			
(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) a $x,\frac{1}{4},z$	(4) b $\frac{1}{4},y,z$

Figure 1.4.2.2
General-position and symmetry-operations blocks as given in the space-group tables for space group *Fmm*2 (42). The numbering scheme of the entries in the different symmetry-operations blocks follows that of the general position.

coset representatives of $P2_1/c$ with respect to its translation subgroup.

For space groups with conventional *centred* cells, there are several (2, 3 or 4) blocks of symmetry operations: one block for each of the translations listed below the subheading 'Coordinates'. Consider, for example, the four symmetry-operations blocks of the space group *Fmm*2 (42) reproduced in Fig. 1.4.2.2. They correspond to the four sets of coordinate triplets of the general position obtained by the translations $t(0,0,0)$, $t(0,\frac{1}{2},\frac{1}{2})$, $t(\frac{1}{2},0,\frac{1}{2})$ and $t(\frac{1}{2},\frac{1}{2},0)$, *cf.* Fig. 1.4.2.2. The numbering scheme of the entries in the different symmetry-operations blocks follows that of the general position. For example, the geometric description of entry (4) in the symmetry-operations block under the heading 'For $(\frac{1}{2},\frac{1}{2},0)+$ set' of *Fmm*2 corresponds to the coordinate triplet $\overline{x}+\frac{1}{2},y+\frac{1}{2},z$, which is obtained by adding $t(\frac{1}{2},\frac{1}{2},0)$ to the translation part of the printed coordinate triplet (4) $\overline{x},y,z$ (*cf.* Fig. 1.4.2.2).

1.4.2.2. Seitz symbols of symmetry operations

Apart from the notation for the geometric interpretation of the matrix–column representation of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$ discussed in detail in the previous section, there is another notation which has been adopted and is widely used by solid-state physicists and chemists. This is the so-called Seitz notation $\{\boldsymbol{R}|\boldsymbol{v}\}$ introduced by Seitz in a series of papers on the matrix-algebraic development of crystallographic groups (Seitz, 1935).

Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ reflect the fact that space-group operations are affine mappings and are essentially shorthand descriptions of the matrix–column representations of the symmetry operations of the space groups. They consist of two parts: a rotation (or linear) part $\boldsymbol{R}$ and a translation part $\boldsymbol{v}$. The Seitz symbol is specified between braces and the rotational and the translational parts are separated by a vertical line. The translation parts $\boldsymbol{v}$ correspond exactly to the columns $\boldsymbol{w}$ of the coordinate triplets of the general-position blocks of the space-group tables. The rotation parts $\boldsymbol{R}$ consist of symbols that specify (i) the type and the order of the symmetry operation, and (ii) the orientation of the corresponding symmetry element with respect to the basis. The orientation is denoted by the direction of the axis for rotations or rotoinversions, or the direction of the normal to reflection planes. (Note that in the latter case this is different from the way the orientation of reflection planes is given in the symmetry-operations block.)

The linear parts of Seitz symbols are denoted in many different ways in the literature (Litvin & Kopsky, 2011). According to the conventions approved by the Commission of Crystallographic Nomenclature of the International Union of Crystallography (Glazer *et al.*, 2014) the symbol $\boldsymbol{R}$ is 1 and $\bar{1}$ for the identity and the inversion, m for reflections, the symbols 2, 3, 4 and 6 are used for rotations and $\bar{3}$, $\bar{4}$ and $\bar{6}$ for rotoinversions. For rotations and rotoinversions of order higher than 2, a superscript + or − is used to indicate the sense of the rotation. Subscripts of the symbols $\boldsymbol{R}$ denote the characteristic direction of the operation: for example, the subscripts 100, 010 and $1\bar{1}0$ refer to the directions [100], [010] and $[1\bar{1}0]$, respectively.

Examples

(*a*) Consider the coordinate triplets of the general positions of $P2_12_12$ (18):

(1) x, y, z (2) $\bar{x}, \bar{y}, z$ (3) $\overline{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$ (4) $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, \bar{z}$

The corresponding geometric interpretations of the symmetry operations are given by

(1) 1 (2) 2 0, 0, z (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4}, y, 0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

In Seitz notation the symmetry operations are denoted by

(1) $\{1|0\}$ (2) $\{2_{001}|0\}$ (3) $\{2_{010}|\frac{1}{2},\frac{1}{2},0\}$ (4) $\{2_{100}|\frac{1}{2},\frac{1}{2},0\}$

(*b*) Similarly, the symmetry operations corresponding to the general-position coordinate triplets of $P2_1/c$ (14), *cf.* Fig. 1.4.2.1, in Seitz notation are given as

(1) $\{1|0\}$ (2) $\{2_{010}|0,\frac{1}{2},\frac{1}{2}\}$ (3) $\{\bar{1}|0\}$ (4) $\{m_{010}|0,\frac{1}{2},\frac{1}{2}\}$

The linear parts $\boldsymbol{R}$ of the Seitz symbols of the space-group symmetry operations are shown in Tables 1.4.2.1–1.4.2.3. Each symbol $\boldsymbol{R}$ is specified by the shorthand notation of its (3×3) matrix representation (also known as the *Jones' faithful representation symbol*, *cf.* Bradley & Cracknell, 1972), the type of symmetry operation and its orientation as described in the corresponding symmetry-operations block of the space-group tables of this volume. The sequence of $\boldsymbol{R}$ symbols in Table 1.4.2.1 corresponds to the numbering scheme of the general-position coordinate triplets of the space groups of the $m\bar{3}m$ crystal class, while those of Table 1.4.2.2 and Table 1.4.2.3 correspond to the general-position sequences of the space groups of 6/*mmm* and $\bar{3}m$ (rhombohedral axes) crystal classes, respectively.

The same symbols $\boldsymbol{R}$ can be used for the construction of Seitz symbols for the symmetry operations of subperiodic layer and rod groups (Litvin & Kopsky, 2014), and magnetic groups, or for the designation of the symmetry operations of the point groups of space groups. [One should note that the Seitz symbols applied in

Table 1.4.2.1
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for space-group symmetry operations of cubic, tetragonal, orthorhombic, monoclinic and triclinic crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction.

IT A description				
No.	Coordinate triplet	Type	Orientation	Seitz symbol
1	x, y, z	1		1
2	$\bar{x}, \bar{y}, z$	2	$0, 0, z$	2_{001}
3	$\bar{x}, y, \bar{z}$	2	$0, y, 0$	2_{010}
4	$x, \bar{y}, \bar{z}$	2	$x, 0, 0$	2_{100}
5	z, x, y	3^+	x, x, x	3^+_{111}
6	$z, \bar{x}, \bar{y}$	3^+	$\bar{x}, x, \bar{x}$	$3^+_{11\bar{1}}$
7	$\bar{z}, \bar{x}, y$	3^+	$x, \bar{x}, \bar{x}$	$3^+_{1\bar{1}\bar{1}}$
8	$\bar{z}, x, \bar{y}$	3^+	$\bar{x}, \bar{x}, x$	$3^+_{\bar{1}\bar{1}1}$
9	y, z, x	3^-	x, x, x	3^-_{111}
10	$\bar{y}, z, \bar{x}$	3^-	$x, \bar{x}, \bar{x}$	$3^-_{1\bar{1}\bar{1}}$
11	$y, \bar{z}, \bar{x}$	3^-	$\bar{x}, \bar{x}, x$	$3^-_{\bar{1}\bar{1}1}$
12	$\bar{y}, \bar{z}, x$	3^-	$\bar{x}, x, \bar{x}$	$3^-_{\bar{1}1\bar{1}}$
13	$y, x, \bar{z}$	2	$x, x, 0$	2_{110}
14	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
15	$y, \bar{x}, z$	4^-	$0, 0, z$	4^-_{001}
16	$\bar{y}, x, z$	4^+	$0, 0, z$	4^+_{001}
17	$x, z, \bar{y}$	4^-	$x, 0, 0$	$4^-_{\bar{1}00}$
18	$\bar{x}, z, y$	2	$0, y, y$	2_{011}
19	$\bar{x}, \bar{z}, \bar{y}$	2	$0, y, \bar{y}$	$2_{01\bar{1}}$
20	$x, \bar{z}, y$	4^+	$x, 0, 0$	4^+_{100}
21	$z, y, \bar{x}$	4^+	$0, y, 0$	4^+_{010}
22	$z, \bar{y}, x$	2	$x, 0, x$	2_{101}
23	$\bar{z}, y, x$	4^-	$0, y, 0$	4^-_{010}
24	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
25	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
26	$x, y, \bar{z}$	m	$x, y, 0$	m_{001}
27	$x, \bar{y}, z$	m	$x, 0, z$	m_{010}
28	$\bar{x}, y, z$	m	$0, y, z$	m_{100}
29	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^+$	x, x, x	$\bar{3}^+_{111}$
30	$\bar{z}, x, y$	$\bar{3}^+$	$\bar{x}, x, \bar{x}$	$\bar{3}^+_{11\bar{1}}$
31	$z, x, \bar{y}$	$\bar{3}^+$	$x, \bar{x}, \bar{x}$	$\bar{3}^+_{1\bar{1}\bar{1}}$
32	$z, \bar{x}, y$	$\bar{3}^+$	$\bar{x}, \bar{x}, x$	$\bar{3}^+_{\bar{1}\bar{1}1}$
33	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^-$	x, x, x	$\bar{3}^-_{111}$
34	$y, \bar{z}, x$	$\bar{3}^-$	$x, \bar{x}, \bar{x}$	$\bar{3}^-_{1\bar{1}\bar{1}}$
35	$\bar{y}, z, x$	$\bar{3}^-$	$\bar{x}, \bar{x}, x$	$\bar{3}^-_{\bar{1}\bar{1}1}$
36	$y, z, \bar{x}$	$\bar{3}^-$	$\bar{x}, x, \bar{x}$	$\bar{3}^-_{\bar{1}1\bar{1}}$
37	$\bar{y}, \bar{x}, z$	m	$x, \bar{x}, z$	m_{110}
38	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
39	$\bar{y}, x, \bar{z}$	$\bar{4}^-$	$0, 0, z$	$\bar{4}^-_{001}$
40	$y, \bar{x}, \bar{z}$	$\bar{4}^+$	$0, 0, z$	$\bar{4}^+_{001}$
41	$\bar{x}, \bar{z}, y$	$\bar{4}^-$	$x, 0, 0$	$\bar{4}^-_{\bar{1}00}$
42	$x, \bar{z}, \bar{y}$	m	$x, y, \bar{y}$	m_{011}
43	x, z, y	m	x, y, y	$m_{01\bar{1}}$
44	$\bar{x}, z, \bar{y}$	$\bar{4}^+$	$x, 0, 0$	$\bar{4}^+_{100}$
45	$\bar{z}, \bar{y}, x$	$\bar{4}^+$	$0, y, 0$	$\bar{4}^+_{010}$
46	$\bar{z}, y, \bar{x}$	m	$\bar{x}, y, x$	m_{101}
47	$z, \bar{y}, \bar{x}$	$\bar{4}^-$	$0, y, 0$	$\bar{4}^-_{010}$
48	z, y, x	m	x, y, x	$m_{\bar{1}01}$

Table 1.4.2.2
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for space-group symmetry operations of hexagonal and trigonal crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction.

IT A description				
No.	Coordinate triplet	Type	Orientation	Seitz symbol
1	x, y, z	1		1
2	$\bar{y}, x-y, z$	3^+	$0, 0, z$	3^+_{001}
3	$\bar{x}+y, \bar{x}, z$	3^-	$0, 0, z$	3^-_{001}
4	$\bar{x}, \bar{y}, z$	2	$0, 0, z$	2_{001}
5	$y, \bar{x}+y, z$	6^-	$0, 0, z$	6^-_{001}
6	$x-y, x, z$	6^+	$0, 0, z$	6^+_{001}
7	$y, x, \bar{z}$	2	$x, x, 0$	2_{110}
8	$x-y, \bar{y}, \bar{z}$	2	$x, 0, 0$	2_{100}
9	$\bar{x}, \bar{x}+y, \bar{z}$	2	$0, y, 0$	2_{010}
10	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
11	$\bar{x}+y, y, \bar{z}$	2	$x, 2x, 0$	2_{120}
12	$x, x-y, \bar{z}$	2	$2x, x, 0$	2_{210}
13	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
14	$y, \bar{x}+y, \bar{z}$	$\bar{3}^+$	$0, 0, z$	$\bar{3}^+_{001}$
15	$x-y, x, \bar{z}$	$\bar{3}^-$	$0, 0, z$	$\bar{3}^-_{001}$
16	$x, y, \bar{z}$	m	$x, y, 0$	m_{001}
17	$\bar{y}, x-y, \bar{z}$	$\bar{6}^-$	$0, 0, z$	$\bar{6}^-_{001}$
18	$\bar{x}+y, \bar{x}, \bar{z}$	$\bar{6}^+$	$0, 0, z$	$\bar{6}^+_{001}$
19	$\bar{y}, \bar{x}, z$	m	$x, \bar{x}, z$	m_{110}
20	$\bar{x}+y, y, z$	m	$x, 2x, z$	m_{100}
21	$x, x-y, z$	m	$2x, x, z$	m_{010}
22	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
23	$x-y, \bar{y}, z$	m	$x, 0, z$	m_{120}
24	$\bar{x}, \bar{x}+y, z$	m	$0, y, z$	m_{210}

Table 1.4.2.3
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for symmetry operations of rhombohedral space groups (rhombohedral-axes setting)

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction.

IT A description				
No.	Coordinate triplet	Type	Orientation	Seitz symbol
1	x, y, z	1		1
2	z, x, y	3^+	x, x, x	3^+_{111}
3	y, z, x	3^-	x, x, x	3^-_{111}
4	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
5	$\bar{y}, \bar{x}, \bar{z}$	2	$x, \bar{x}, 0$	$2_{1\bar{1}0}$
6	$\bar{x}, \bar{z}, \bar{y}$	2	$0, y, \bar{y}$	$2_{01\bar{1}}$
7	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
8	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^+$	x, x, x	$\bar{3}^+_{111}$
9	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^-$	x, x, x	$\bar{3}^-_{111}$
10	z, y, x	m	x, y, x	$m_{\bar{1}01}$
11	y, x, z	m	x, x, z	$m_{1\bar{1}0}$
12	x, z, y	m	x, y, y	$m_{01\bar{1}}$

Table 1.4.2.4
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for plane-group symmetry operations of oblique, rectangular and square crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction (if applicable).

IT A description				
No.	Coordinate doublet	Type	Orientation	Seitz symbol
1	x, y	1		1
2	$\bar{x}, \bar{y}$	2		2
3	$\bar{y}, x$	4^+		4^+
4	$y, \bar{x}$	4^-		4^-
5	$\bar{x}, y$	m	$0, y$	m_{10}
6	$x, \bar{y}$	m	$x, 0$	m_{01}
7	y, x	m	x, x	$m_{1\bar{1}}$
8	$\bar{y}, \bar{x}$	m	$x, \bar{x}$	m_{11}

Table 1.4.2.5
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ for plane-group symmetry operations of the hexagonal crystal system

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction (if applicable).

IT A description				
No.	Coordinate doublet	Type	Orientation	Seitz symbol
1	x, y	1		1
2	$\bar{y}, x-y$	3^+		3^+
3	$\bar{x}+y, \bar{x}$	3^-		3^-
4	$\bar{x}, \bar{y}$	2		2
5	$y, \bar{x}+y$	6^-		6^-
6	$x-y, x$	6^+		6^+
7	$\bar{y}, \bar{x}$	m	$x, \bar{x}$	m_{11}
8	$\bar{x}+y, y$	m	$x, 2x$	m_{10}
9	$x, x-y$	m	$2x, x$	m_{01}
10	y, x	m	x, x	$m_{1\bar{1}}$
11	$x-y, \bar{y}$	m	$x, 0$	m_{12}
12	$\bar{x}, \bar{x}+y$	m	$0, y$	m_{21}

the first and second editions of *IT* E and in the IUCr e-book on magnetic groups (Litvin, 2012) differ from the standard symbols adopted by the Commission of Crystallographic Nomenclature.]

The Seitz symbols for plane groups are constructed following similar rules to those for space groups. The rotation part $\boldsymbol{R}$ is 1 for the identity, m for reflections, and 2, 3, 4 and 6 are used for rotations. The orientation of a reflection line is specified by a subscript indicating the direction of its 'normal'. Obviously, the direction indicators are of no relevance for the rotation points. The linear parts $\boldsymbol{R}$ of the Seitz symbols of the plane-group symmetry operations are shown in Tables 1.4.2.4 and 1.4.2.5. Each symbol $\boldsymbol{R}$ is specified by the shorthand notation of its (2×2) matrix representation, the type of symmetry operation and, if applicable, its orientation as described in the corresponding symmetry-operations block of the plane-group tables of this volume. The sequence of $\boldsymbol{R}$ symbols in Table 1.4.2.4 corresponds to the numbering scheme of the general-position coordinate doublets of the plane group *p*4*mm*, while those of Table 1.4.2.5 correspond to the general-position sequence of the plane group *p*6*mm*. The same symbols $\boldsymbol{R}$ can be used for the construction of Seitz symbols for the symmetry operations of subperiodic frieze groups (Litvin & Kopsky, 2014).

As illustrated in the examples above, zero translations are normally specified by a single zero in the Seitz symbols, but in cases where it is unclear whether the symbol refers to a space- or a plane-group symmetry operation, an explicit indication of the components of the translation vector is recommended.

From the description given above, it is clear that Seitz symbols can be considered as shorthand modifications of the matrix–column presentation $(\boldsymbol{W}, \boldsymbol{w})$ of symmetry operations discussed in detail in Chapter 1.2: the translation parts of $\{\boldsymbol{R}|\boldsymbol{v}\}$ and $(\boldsymbol{W}, \boldsymbol{w})$ coincide, while the different (3×3) matrices $\boldsymbol{W}$ are represented by the symbols $\boldsymbol{R}$ shown in Tables 1.4.2.1–1.4.2.3. As a result, the expressions for the product and the inverse of symmetry operations in Seitz notation are rather similar to those of the matrix–column pairs $(\boldsymbol{W}, \boldsymbol{w})$ discussed in detail in Chapter 1.2:

(*a*) product of symmetry operations:

$$\{\boldsymbol{R}_1|\boldsymbol{v}_1\}\{\boldsymbol{R}_2|\boldsymbol{v}_2\} = \{\boldsymbol{R}_1\boldsymbol{R}_2|\boldsymbol{R}_1\boldsymbol{v}_2 + \boldsymbol{v}_1\};$$

(*b*) inverse of a symmetry operation:

$$\{\boldsymbol{R}|\boldsymbol{v}\}^{-1} = \{\boldsymbol{R}^{-1}| - \boldsymbol{R}^{-1}\boldsymbol{v}\}.$$

Similarly, the action of a symmetry operation $\{\boldsymbol{R}|\boldsymbol{v}\}$ on the column of point coordinates $\boldsymbol{x}$ is given by $\{\boldsymbol{R}|\boldsymbol{v}\}\boldsymbol{x} = \boldsymbol{R}\boldsymbol{x} + \boldsymbol{v}$ [*cf.* Chapter 1.2, equation (1.2.2.4)].

The rotation parts of the Seitz symbols partly resemble the geometric-description symbols of symmetry operations described in Section 1.4.2.1 and listed in the symmetry-operation blocks of the space-group tables of this volume: $\boldsymbol{R}$ contains the information on the type and order of the symmetry operation, and its characteristic direction. The Seitz symbols do not *directly* indicate the location of the symmetry operation, nor its glide or screw component, if any.

1.4.2.3. Symmetry operations and the general position

The classifications of space groups introduced in Chapter 1.3 allow one to reduce the practically unlimited number of possible space groups to a finite number of space-group types. However, each individual space-group type still consists of an infinite number of symmetry operations generated by the set of all translations of the space group. A practical way to represent the symmetry operations of space groups is based on the coset decomposition of a space group with respect to its translation subgroup, which was introduced and discussed in Section 1.3.3.2. For our further considerations, it is important to note that the listings of the general position in the space-group tables can be interpreted in two ways:

(i) Each of the numbered entries lists the coordinate triplets of an image point of a starting point with coordinates x, y, z under a symmetry operation of the space group. This feature of the general position will be discussed in detail in Section 1.4.4.

(ii) Each of the numbered entries of the general position lists a symmetry operation of the space group by the shorthand notation of its matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ (*cf.* Section 1.2.2.1). This fact is not as obvious as the more 'crystallographic' aspect described under (i), but its importance becomes evident from the following discussion, where it is shown how to extract the full analytical symmetry information of space groups from the general-position data in the space-group tables of Chapter 2.3.

With reference to a conventional coordinate system, the set of symmetry operations $\{W\}$ of a space group $\mathcal{G}$ is described by the

Table 1.4.2.6
Right coset decomposition of space group $P2_1/c$, No. 14 (unique axis b, cell choice 1) with respect to the normal subgroup of translations $\mathcal{T}$

The numbers u_1, u_2 and u_3 are positive or negative integers.

x	y	z	$\bar{x}$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}$	$\bar{z}$	x	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
$x+1$	y	z	$\bar{x}+1$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}$	$\bar{z}$	$x+1$	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
$x+2$	y	z	$\bar{x}+2$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}$	$\bar{z}$	$x+2$	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	$y+1$	z	$\bar{x}$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}+1$	$\bar{z}$	x	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
$x+1$	$y+1$	z	$\bar{x}+1$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}+1$	$\bar{z}$	$x+1$	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
$x+2$	$y+1$	z	$\bar{x}+2$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}+1$	$\bar{z}$	$x+2$	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	$y+2$	z	$\bar{x}$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}+2$	$\bar{z}$	x	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
$x+1$	$y+2$	z	$\bar{x}+1$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}+2$	$\bar{z}$	$x+1$	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
$x+2$	$y+2$	z	$\bar{x}+2$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}+2$	$\bar{z}$	$x+2$	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	y	$z+1$	$\bar{x}$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}$	$\bar{y}$	$\bar{z}+1$	x	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
$x+1$	y	$z+1$	$\bar{x}+1$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+1$	$\bar{y}$	$\bar{z}+1$	$x+1$	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
$x+2$	y	$z+1$	$\bar{x}+2$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+2$	$\bar{y}$	$\bar{z}+1$	$x+2$	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	$y+1$	$z+1$	$\bar{x}$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}$	$\bar{y}+1$	$\bar{z}+1$	x	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
$x+1$	$y+1$	$z+1$	$\bar{x}+1$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+1$	$\bar{y}+1$	$\bar{z}+1$	$x+1$	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
$x+2$	$y+1$	$z+1$	$\bar{x}+2$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+2$	$\bar{y}+1$	$\bar{z}+1$	$x+2$	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
$x+u_1$	$y+u_2$	$z+u_3$	$\bar{x}+u_1$	$y+u_2+\frac{1}{2}$	$\bar{z}+u_3+\frac{1}{2}$	$\bar{x}+u_1$	$\bar{y}+u_2$	$\bar{z}+u_3$	$x+u_1$	$\bar{y}+u_2+\frac{1}{2}$	$z+u_3+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	

set of matrix–column pairs $\{(\boldsymbol{W}, \boldsymbol{w})\}$. The set $\mathcal{T}_\mathcal{G} = \{(\boldsymbol{I}, \boldsymbol{t})\}$ of all translations forms the *translation subgroup* $\mathcal{T}_\mathcal{G} \lhd \mathcal{G}$, which is a normal subgroup of $\mathcal{G}$ of finite index $[i]$. If $(\boldsymbol{W}, \boldsymbol{w})$ is a fixed symmetry operation, then all the products $\mathcal{T}_\mathcal{G}(\boldsymbol{W}, \boldsymbol{w}) = \{(\boldsymbol{I}, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w})\} = \{(\boldsymbol{W}, \boldsymbol{w} + \boldsymbol{t})\}$ of translations with $(\boldsymbol{W}, \boldsymbol{w})$ have the same rotation part $\boldsymbol{W}$. Conversely, every symmetry operation $\boldsymbol{W}$ of $\mathcal{G}$ with the same matrix part $\boldsymbol{W}$ is represented in the set $\mathcal{T}_\mathcal{G}(\boldsymbol{W}, \boldsymbol{w})$. The infinite set of symmetry operations $\mathcal{T}_\mathcal{G}(\boldsymbol{W}, \boldsymbol{w})$ is called a coset of the right coset decomposition of $\mathcal{G}$ with respect to $\mathcal{T}_\mathcal{G}$, and $(\boldsymbol{W}, \boldsymbol{w})$ its coset representative. In this way, the symmetry operations of $\mathcal{G}$ can be distributed into a finite set of infinite cosets, the elements of which are obtained by the combination of a coset representative $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ and the infinite set $\mathcal{T}_\mathcal{G} = \{(\boldsymbol{I}, \boldsymbol{t})\}$ of translations (*cf.* Section 1.3.3.2):

$$\mathcal{G} = \mathcal{T}_\mathcal{G} \cup \mathcal{T}_\mathcal{G}(\boldsymbol{W}_2, \boldsymbol{w}_2) \cup \cdots \cup \mathcal{T}_\mathcal{G}(\boldsymbol{W}_m, \boldsymbol{w}_m) \cup \cdots \cup \mathcal{T}_\mathcal{G}(\boldsymbol{W}_i, \boldsymbol{w}_i), \tag{1.4.2.1}$$

where $(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{I}, \boldsymbol{o})$ is omitted. Obviously, the coset representatives $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ of the decomposition $(\mathcal{G} : \mathcal{T}_\mathcal{G})$ represent in a clear and compact way the infinite number of symmetry operations of the space group $\mathcal{G}$. Each coset in the decomposition $(\mathcal{G} : \mathcal{T}_\mathcal{G})$ is characterized by its linear part $\boldsymbol{W}_j$ and its entries differ only by lattice translations. The translations $(\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}_\mathcal{G}$ form the first coset with the identity $(\boldsymbol{I}, \boldsymbol{o})$ as a coset representative. The symmetry operations with rotation part $\boldsymbol{W}_2$ form the second coset *etc*. The number of cosets equals the number of different matrices $\boldsymbol{W}_j$ of the symmetry operations of the space group. This number $[i]$ is always finite and is equal to the order of the point group $\mathcal{P}_\mathcal{G}$ of the space group (*cf.* Section 1.3.3.2).

For each space group, a set of coset representatives $\{(\boldsymbol{W}_j, \boldsymbol{w}_j), 1 \le j \le [i]\}$ of the decomposition $(\mathcal{G} : \mathcal{T}_\mathcal{G})$ is listed under the general-position block of the space-group tables. In general, any element of a coset may be chosen as a coset representative. For convenience, the representatives listed in the space-group tables are always chosen such that the components $w_{j,k}$, $k = 1, 2, 3$, of the translation parts $\boldsymbol{w}_j$ fulfil $0 \le w_{j,k} < 1$ (by subtracting integers). To save space, each matrix–column pair $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ is represented by the corresponding *coordinate triplet* (*cf.* Section 1.2.2.3 for the shorthand notation of matrix–column pairs).

Example

The right coset decomposition of $P2_1/c$, No. 14 (unique axis b, cell choice 1) with respect to its translation subgroup is shown in Table 1.4.2.6. All possible symmetry operations of $P2_1/c$ are distributed into four cosets:

The first column represents the infinitely many translations $t = (\boldsymbol{I}, \boldsymbol{t}) = x + u_1, y + u_2, z + u_3 = \{1|u_1, u_2, u_3\}$ of the translation subgroup $\mathcal{T}$ of $P2_1/c$. The numbers u_1, u_2 and u_3 are positive or negative integers. The identity operation $(\boldsymbol{I}, \boldsymbol{o})$ is usually chosen as a coset representative.

The third coset of the decomposition $(\mathcal{G} : \mathcal{T}_\mathcal{G})$ represents the infinite set of inversions $(-\boldsymbol{I}, \boldsymbol{t}) = \bar{x} + u_1, \bar{y} + u_2, \bar{z} + u_3 = \{\bar{1}|u_1, u_2, u_3\}$ of the space group $P2_1/c$ with inversion centres located at $u_1/2, u_2/2, u_3/2$ (*cf.* Section 1.2.2.4 for the determination of the location of the inversion centres). The inversion in the origin, *i.e.* $\bar{x}, \bar{y}, \bar{z} = \{\bar{1}|0\}$, is taken as a coset representative.

The coset representative of the second coset is the twofold screw rotation $\{2_{010}|0, \frac{1}{2}, \frac{1}{2}\}$ around the line $0, y, \frac{1}{4}$, followed by its infinite combinations with all lattice translations: $\bar{x} + u_1$, $y + \frac{1}{2} + u_2, \bar{z} + \frac{1}{2} + u_3 = \{2_{010}|u_1, \frac{1}{2} + u_2, \frac{1}{2} + u_3\}$. These are twofold screw rotations around the lines $u_1/2, y, u_3/2 + \frac{1}{4}$ with screw components $\begin{pmatrix} 0 \\ \frac{1}{2} + u_2 \\ 0 \end{pmatrix}$.

The symmetry operations of the fourth column represented by $x + u_1$, $\bar{y} + \frac{1}{2} + u_2$, $z + \frac{1}{2} + u_3 = \{m_{010}|u_1, \frac{1}{2} + u_2, \frac{1}{2} + u_3\}$ correspond to glide reflections with glide components $\begin{pmatrix} u_1 \\ 0 \\ \frac{1}{2} + u_3 \end{pmatrix}$ through the (infinite) set of glide planes at $x, \frac{1}{4}, z$;

$x, \frac{3}{4}, z$; $x, \frac{5}{4}, z$; ...; $x, (2u_2+1)/4, z$. As usual, the symmetry operation with $u_1 = u_2 = u_3 = 0$, *i.e.* $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2} = \{m_{010}|0, \frac{1}{2}, \frac{1}{2}\}$, is taken as a coset representative of the coset of glide reflections.

The coordinate triplets of the general-position block of $P2_1/c$ (unique axis b, cell choice 1) (*cf.* Fig. 1.4.2.1) correspond to the coset representatives of the decomposition of the group listed in the first line of Table 1.4.2.6.

When the space group is referred to a primitive basis (which is always done for '*P*' space groups), each coordinate triplet of the general-position block corresponds to one coset of $(\mathcal{G} : \mathcal{T}_\mathcal{G})$, *i.e.* the *multiplicity* of the general position and the number of cosets is the same. If, however, the space group is referred to a centred cell, then the complete set of general-position coordinate triplets is obtained by the combinations of the listed coordinate triplets with the centring translations. In this way, the total number of coordinate triplets per conventional unit cell, *i.e.* the multiplicity of the general position, is given by the product $[i] \times [p]$, where $[i]$ is the index of $\mathcal{T}_\mathcal{G}$ in $\mathcal{G}$ and $[p]$ is the index of the group of integer translations in the group $\mathcal{T}_\mathcal{G}$ of all (integer and centring) translations.

Example

The listing of the general position for the space–group type *Fmm*2 (42) of the space-group tables is reproduced in Fig. 1.4.2.2. The four entries, numbered (1) to (4), are to be taken as they are printed [indicated by (0, 0, 0)+]. The additional 12 more entries are obtained by adding the centring translations $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$ to the translation parts of the printed entries [indicated by $(0, \frac{1}{2}, \frac{1}{2})$+, $(\frac{1}{2}, 0, \frac{1}{2})$+ and $(\frac{1}{2}, \frac{1}{2}, 0)$+, respectively]. Altogether there are 16 entries, which is announced by the multiplicity of the general position, *i.e.* by the first number in the row. (The additional information specified on the left of the general-position block, namely the Wyckoff letter and the site symmetry, will be dealt with in Section 1.4.4.)

1.4.2.4. Additional symmetry operations and symmetry elements

The symmetry operations of a space group are conveniently partitioned into the cosets with respect to the translation subgroup. All operations which belong to the same coset have the same linear part and, if a single operation from a coset is given, all other operations in this coset are obtained by composition with a translation. However, not all symmetry operations in a coset with respect to the translation subgroup are operations of the same type and, furthermore, they may belong to element sets of different symmetry elements. In general, one can distinguish the following cases:

(i) The composition $W' = tW$ of a symmetry operation W with a translation t is an operation of the same type as W, with the same or a different type of symmetry element.

(ii) The composition $W' = tW$ is an operation of a different type to W with the same or a different type of symmetry element.

In order to distinguish the different cases, a closer analysis of the type of a symmetry operation and its symmetry element is required. These types, however, might be obscured by two obstacles:

(1) The origin in the chosen coordinate system might not lie on the geometric element of the symmetry operation. For example, the symmetry operation represented by the coordinate triplet $\bar{x}+1, \bar{y}+1, \bar{z}$ (*cf.* Section 1.4.2.3) is in fact an inversion through the point $1/2, 1/2, 0$ and thus of the same type as the inversion $\{\bar{1}|0\}$ through the origin.

(2) The screw or glide part might not be reduced to a vector within the unit cell. For example, the symmetry operation $\bar{x}, \bar{y}, z+1$, which is a twofold screw rotation 2 (0, 0, 1) 0, 0, z along the c axis, is the composition of the twofold rotation $\bar{x}, \bar{y}, z$ with the lattice translation $t(0, 0, 1)$ along the screw axis. Although the two operations $\bar{x}, \bar{y}, z$ and $\bar{x}, \bar{y}, z+1$ are of different types, they are coaxial equivalents and belong to the element set of the same symmetry element (*cf.* Section 1.2.3).

These issues can be overcome by decomposing the translation part $\boldsymbol{w}$ of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ into an intrinsic translation part $\boldsymbol{w}_g$ which is fixed by the linear part $\boldsymbol{W}$ of W and thus parallel to the geometric element of W, and a location part $\boldsymbol{w}_l$, which is perpendicular to the intrinsic translation part. Note that the subspace of vectors fixed by $\boldsymbol{W}$ and the subspace perpendicular to this space of fixed vectors are complementary subspaces, *i.e.* their dimensions add up to 3, therefore this decomposition is always possible.

The procedure for determining the intrinsic translation part of a symmetry operation is described in Section 1.2.2.4, and is based on the fact that the kth power of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ with linear part $\boldsymbol{W}$ of order k must be a pure translation, *i.e.* $W^k = (\boldsymbol{I}, \boldsymbol{t})$ for some lattice translation $\boldsymbol{t}$. The *intrinsic translation part* of W is then defined as $\boldsymbol{w}_g = \frac{1}{k}\boldsymbol{t}$.

The difference $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{w}_g$ is perpendicular to $\boldsymbol{w}_g$ and it is called the *location part* of $\boldsymbol{w}$. This terminology is justified by the fact that the location part can be reduced to $\boldsymbol{o}$ by an origin shift, *i.e.* the location part indicates whether the origin of the chosen coordinate system lies on the geometric element of W.

The transformation of point coordinates and matrix–column pairs under an origin shift is explained in detail in Sections 1.5.1.3 and 1.5.2.3, and the complete procedure for determining the additional symmetry operations will be discussed in the context of the synoptic tables in Section 1.5.4. In this section we will restrict ourselves to a detailed discussion of two examples which illustrate typical phenomena.

Example 1

Consider a space group of type *Fmm*2 (42). The information on the general position and on the symmetry operations given in the space-group tables are reproduced in Fig. 1.4.2.2. From this information one deduces that coset representatives with respect to the translation subgroup are the identity element $W_1 = x, y, z$, a rotation $W_2 = \bar{x}, \bar{y}, z$ with the c axis as geometric element, a reflection $W_3 = x, \bar{y}, z$ with the plane $x, 0, z$ as geometric element and a reflection $W_4 = \bar{x}, y, z$ with the plane $0, y, z$ as geometric element (with the indices following the numbering in the table).

Composing these coset representatives with the centring translations $t(0, \frac{1}{2}, \frac{1}{2})$, $t(\frac{1}{2}, 0, \frac{1}{2})$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ gives rise to elements in the same cosets, but with different types of symmetry operations and symmetry elements in several cases.

(i) $(0, \frac{1}{2}, \frac{1}{2})$: The composition of the rotation W_2 with $t(0, \frac{1}{2}, \frac{1}{2})$ results in the symmetry operation $\bar{x}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$, which is a twofold screw rotation with screw axis $0, \frac{1}{4}, z$. This means that both the type of the symmetry operation and the location of the geometric element are changed. Composing the reflection W_3 with $t(0, \frac{1}{2}, \frac{1}{2})$ gives the symmetry operation $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$, which is a c glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the b axis relative to the geometric element of W_3. In the composition of W_4 with $t(0, \frac{1}{2}, \frac{1}{2})$, the translation lies

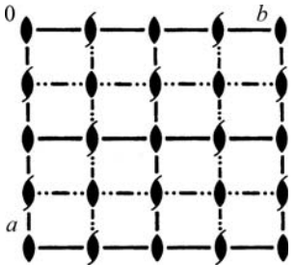

Figure 1.4.2.3
Symmetry-element diagram for space group *Fmm*2 (42) (orthogonal projection along [001]).

in the plane forming the geometric element of W_4. The geometric element of the resulting symmetry operation $\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$ is still the plane $0, y, z$, but the symmetry operation is now an *n* glide, *i.e.* a glide reflection with diagonal glide vector.

(ii) $(\frac{1}{2}, 0, \frac{1}{2})$: Analogous to the first centring translation, the composition of W_2 with $t(\frac{1}{2}, 0, \frac{1}{2})$ results in a twofold screw rotation with screw axis $\frac{1}{4}, 0, z$ as geometric element. The roles of the reflections W_3 and W_4 are interchanged, because the translation vector now lies in the plane forming the geometric element of W_3. Therefore, the composition of W_3 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an *n* glide with the plane $x, 0, z$ as geometric element, whereas the composition of W_4 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is a *c* glide with the plane $\frac{1}{4}, y, z$ as geometric element.

(iii) $(\frac{1}{2}, \frac{1}{2}, 0)$: Because this translation vector lies in the plane perpendicular to the rotation axis of W_2, the composition of W_2 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is still a twofold rotation, *i.e.* a symmetry operation of the same type, but the rotation axis is shifted by $\frac{1}{4}, \frac{1}{4}, 0$ in the *xy* plane to become the axis $\frac{1}{4}, \frac{1}{4}, z$. The composition of W_3 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ results in the symmetry operation $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$, which is an *a* glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the *b* axis relative to the geometric element of W_3. Similarly, the composition of W_4 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is a *b* glide with the plane $\frac{1}{4}, y, z$ as geometric element.

In this example, all additional symmetry operations are listed in the symmetry-operations block of the space-group tables of *Fmm*2 because they are due to compositions of the coset representatives with centring translations.

The additional symmetry operations can easily be recognized in the symmetry-element diagrams (*cf.* Section 1.4.2.5). Fig. 1.4.2.3 shows the symmetry-element diagram of *Fmm*2 for the projection along the *c* axis. One sees that twofold rotation axes alternate with twofold screw axes and that mirror planes alternate with 'double' or *e*-glide planes, *i.e.* glide planes with two glide vectors. For example, the dot–dashed lines at $x=\frac{1}{4}$ and $x=\frac{3}{4}$ in Fig. 1.4.2.3 represent the *b* and *c* glides with normal vector along the *a* axis [for a discussion of *e*-glide notation, see Sections 1.2.3 and 2.1.2, and de Wolff *et al.*, 1992].

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			
8	*g* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
		(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

Symmetry operations

(1) 1	(2) 2 0,0,*z*	(3) 4^+ 0,0,*z*	(4) 4^- 0,0,*z*
(5) *m* *x*,0,*z*	(6) *m* 0,*y*,*z*	(7) *m* *x*,$\bar{x}$,*z*	(8) *m* *x*,*x*,*z*

Figure 1.4.2.4
General-position and symmetry-operations blocks as given in the space-group tables for space group *P*4*mm* (99).

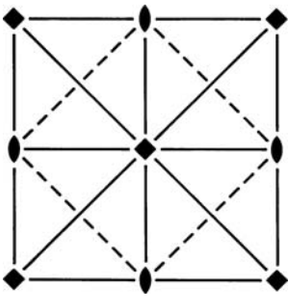

Figure 1.4.2.5
Symmetry-element diagram for space group *P*4*mm* (99) (orthogonal projection along [001]).

Example 2

In a space group of type *P*4*mm* (99), representatives of the space group with respect to the translation subgroup are the powers of a fourfold rotation and reflections with normal vectors along the *a* and the *b* axis and along the diagonals [110] and $[1\bar{1}0]$ (*cf.* Fig. 1.4.2.4).

In this case, additional symmetry operations occur although there are no centring translations. Consider for example the reflection W_8 with the plane x, x, z as geometric element. Composing this reflection with the translation $t(1, 0, 0)$ gives rise to the symmetry operation represented by $y+1, x, z$. This operation maps a point with coordinates $x+\frac{1}{2}, x, z$ to $x+1, x+\frac{1}{2}, z$ and is thus a glide reflection with the plane $x+\frac{1}{2}, x, z$ as geometric element and $(\frac{1}{2}, \frac{1}{2}, 0)$ as glide vector. In a similar way, composing the other diagonal reflection with translations yields further glide reflections.

These glide reflections are symmetry operations which are not listed in the symmetry-operations block, although they are clearly of a different type to the operations given there. However, in the symmetry-element diagram as shown in Fig. 1.4.2.5, the corresponding symmetry elements are displayed as diagonal dashed lines which alternate with the solid diagonal lines representing the diagonal reflections.

1.4.2.5. Space-group diagrams

In the space-group tables of Chapter 2.3, for each space group there are at least two diagrams displaying the symmetry (there are more diagrams for space groups of low symmetry). The *symmetry-element* diagram displays the location and orientation of the symmetry elements of the space group. The *general-position* diagrams show the arrangement of a set of symmetry-equivalent points of the general position. Because of the periodicity of the arrangements, the presentation of the contents of one unit cell is sufficient. Both types of diagrams are orthogonal projections of the space-group unit cell onto the plane of projection along a basis vector of the conventional crystallographic coordinate system. The symmetry elements of triclinic, monoclinic and orthorhombic groups are shown in three different projections along the basis vectors.

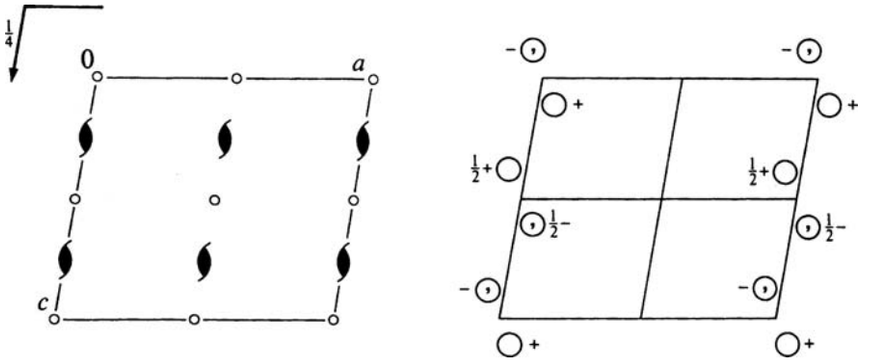

Figure 1.4.2.6
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2_1/c$, No. 14 (unique axis b, cell choice 1).

The thin lines outlining the projection are the traces of the side planes of the unit cell.

Detailed explanations of the diagrams of space groups are found in Section 2.1.3.6. In this section, after a very brief introduction to the diagrams, we will focus mainly on certain important but very often overlooked features of the diagrams.

Symmetry-element diagram

The graphical symbols of the symmetry elements used in the diagrams are explained in Section 2.1.2. The heights along the projection direction above the plane of the diagram are indicated for rotation or screw axes and mirror or glide planes parallel to the projection plane, for rotoinversion axes and inversion centres. The heights (if different from zero) are given as fractions of the shortest translation vector along the projection direction. In Fig. 1.4.2.6 (left) the symmetry elements of $P2_1/c$ (unique axis b, cell choice 1) are represented graphically in a projection of the unit cell along the monoclinic axis **b**. The directions of the basis vectors **c** and **a** can be read directly from the figure. The origin (upper left corner of the unit cell) lies on a centre of inversion indicated by a small open circle. The black lenticular symbols with tails represent the twofold screw axes parallel to **b**. The c-glide plane at height $\frac{1}{4}$ along **b** is shown as a bent arrow with the arrowhead pointing along **c**.

The crystallographic symmetry operations are visualized geometrically by the related symmetry elements. Whereas the symmetry element of a symmetry operation is uniquely defined, more than one symmetry operation may belong to the same symmetry element (*cf.* Section 1.2.3). The following examples illustrate some important features of the diagrams related to the fact that the symmetry-element symbols that are displayed visualize all symmetry operations that belong to the element sets of the symmetry elements.

Examples

(1) *Visualization of the twofold screw rotations of* $P2_1/c$ (Fig. 1.4.2.6). The second coset of the decomposition of $P2_1/c$ with respect to its translation subgroup shown in Table 1.4.2.6 is formed by the infinite set of twofold screw rotations represented by the coordinate triplets $\bar{x}+u_1$, $y+\frac{1}{2}+u_2$, $\bar{z}+\frac{1}{2}+u_3$ (where u_1, u_2, u_3 are integers). To analyse how these symmetry operations are visualized, it is convenient to consider two special cases:

(i) $u_2 = 0$, *i.e.* $\bar{x}+u_1,\ y+\frac{1}{2},\ \bar{z}+\frac{1}{2}+u_3 = \{2_{010}|u_1, \frac{1}{2}, \frac{1}{2}+u_3\}$; these operations correspond to twofold screw rotations around the infinitely many screw axes parallel to the line $0, y, \frac{1}{4}$, *i.e.* around the lines $u_1/2, y, u_3/2+\frac{1}{4}$. The symbols of the symmetry elements (*i.e.* of the twofold screw axes) located in the unit cell at $0, y, \frac{1}{4}$; $0, y, \frac{3}{4}$; $\frac{1}{2}, y, \frac{1}{4}$; $\frac{1}{2}, y, \frac{3}{4}$ (and the translationally equivalent $1, y, \frac{1}{4}$ and $1, y, \frac{3}{4}$) are shown in the symmetry-element diagram (Fig. 1.4.2.6);

(ii) $u_1 = u_3 = 0$, *i.e.* $\bar{x},\ y+\frac{1}{2}+u_2,\ \bar{z}+\frac{1}{2} = \{2_{010}|0, \frac{1}{2}+u_2, \frac{1}{2}\}$; these symmetry operations correspond to screw rotations around the line $0, y, \frac{1}{4}$ with screw components $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots$, *i.e.* with a screw component $\frac{1}{2}$ to which all lattice translations parallel to the screw axis are added. These operations, infinite in number, share the same geometric element, *i.e.* they form the element set of the same symmetry element, and geometrically they are represented just by one graphical symbol on the symmetry-element diagrams located exactly at $0, y, \frac{1}{4}$.

(iii) The rest of the symmetry operations in the coset, *i.e.* those with the translation parts $\begin{pmatrix} u_1 \\ \frac{1}{2}+u_2 \\ \frac{1}{2}+u_3 \end{pmatrix}$, are combinations of the two special cases above.

(2) *Inversion centres of* $P2_1/c$ (Fig. 1.4.2.6). The element set of an inversion centre consists of only one symmetry operation, *viz.* the inversion through the point located at the centre. In other words, to each inversion centre displayed on a symmetry-element diagram there corresponds one symmetry operation of inversion. The infinitely many inversions $(-\boldsymbol{I}, \boldsymbol{t}) = \bar{x}+u_1, \bar{y}+u_2, \bar{z}+u_3 = \{\bar{1}|u_1, u_2, u_3\}$ of $P2_1/c$ are located at points $u_1/2$, $u_2/2$, $u_3/2$. Apart from translational equivalence, there are eight centres located in the unit cell: four at $y = 0$, namely at 0, 0, 0; $\frac{1}{2}$, 0, 0; 0, 0, $\frac{1}{2}$; $\frac{1}{2}$, 0, $\frac{1}{2}$ and four at height $\frac{1}{2}$ of b. It is important to note that only inversion centres at $y = 0$ are indicated on the diagram.

A similar rule is applied to all pairs of symmetry elements of the same type (such as *e.g.* twofold rotation axes, planes *etc.*) whose heights differ by $\frac{1}{2}$ of the shortest lattice direction along the projection direction. For example, the c-glide plane symbol in Fig. 1.4.2.6 with the fraction $\frac{1}{4}$ next to it represents not only the c-glide plane located at height $\frac{1}{4}$ but also the one at height $\frac{3}{4}$.

(3) *Glide reflections visualized by mirror planes*. As discussed in Section 1.2.3, the element set of a mirror or glide plane consists of a defining operation and all its coplanar equivalents (*cf.* Table 1.2.3.1). The corresponding symmetry element is a mirror plane if among the infinite set of the coplanar glide reflections there is one with zero glide vector. Thus, the symmetry element is a mirror plane and

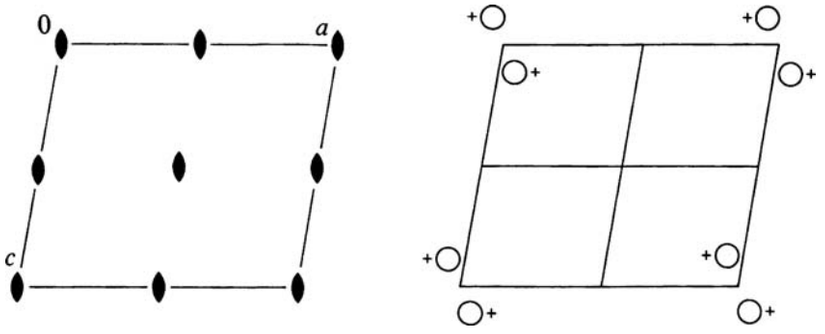

Figure 1.4.2.7
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2$, No. 3 (unique axis b, cell choice 1).

the graphical symbol for a mirror plane is used for its representation on the symmetry-element diagrams of the space groups. For example, the mirror plane $0, y, z$ shown on the symmetry-element diagram of $Fmm2$ (42), *cf.* Fig. 1.4.2.3, represents all glide reflections of the element set of the defining operation $0, y, z$ [symmetry operation (4) of the general-position $(0, 0, 0)+$ set, *cf.* Fig. 1.4.2.2], including the n-glide reflection $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ [entry (4) of the general-position $(0, \frac{1}{2}, \frac{1}{2})+$ set]. In a similar way, the graphical symbols of the mirror planes $x, 0, z$ also represent the n-glide reflections $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ [entry (3) of the general-position $(\frac{1}{2}, 0, \frac{1}{2})+$ set] of $Fmm2$.

General-position diagram

The graphical presentations of the space-group symmetries provided by the general-position diagrams consist of a set of general-position points which are symmetry equivalent under the symmetry operations of the space group. Starting with a point in the upper left corner of the unit cell, indicated by an open circle with a sign '+', all the displayed points inside and near the unit cell are images of the starting point under some symmetry operation of the space group. Because of the one-to-one correspondence between the image points and the symmetry operations, the number of general-position points in the unit cell (excluding the points that are equivalent by integer translations) equals the multiplicity of the general position. The coordinates of the points in the projection plane can be read directly from the diagram. For all systems except cubic, only one parameter is necessary to describe the height along the projection direction. For example, if the height of the starting point above the projection plane is indicated by a '+' sign, then signs '+', '−' or their combinations with fractions (*e.g.* $\frac{1}{2}+$, $\frac{1}{2}-$ *etc.*) are used to specify the heights of the image points. A circle divided by a vertical line represents two points with different coordinates along the projection direction but identical coordinates in the projection plane. A comma ',' in the circle indicates an image point obtained by a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ of the second kind [*i.e.* with $\det(\boldsymbol{W}) = -1$, *cf.* Section 1.2.2].

Example

The general-position diagram of $P2_1/c$ (unique axis b, cell choice 1) is shown in Fig. 1.4.2.6 (right). The open circles indicate the location of the four symmetry-equivalent points of the space group within the unit cell along with additional eight translation-equivalent points to complete the presentation. The circles with a comma inside indicate the image points generated by operations of the second kind – inversions and glide planes in the present case. The fractions and signs close to the circles indicate their heights in units of b of the symmetry-equivalent points along the monoclinic axis. For example, $\frac{1}{2}-$ is a shorthand notation for $\frac{1}{2} - y$.

Notes:

(1) The close relation between the symmetry-element and the general-position diagrams is obvious. For example, the points shown on the general-position diagram are images of a general-position point under the action of the space-group symmetry operations displayed by the corresponding symmetry elements on the symmetry-element diagram. With

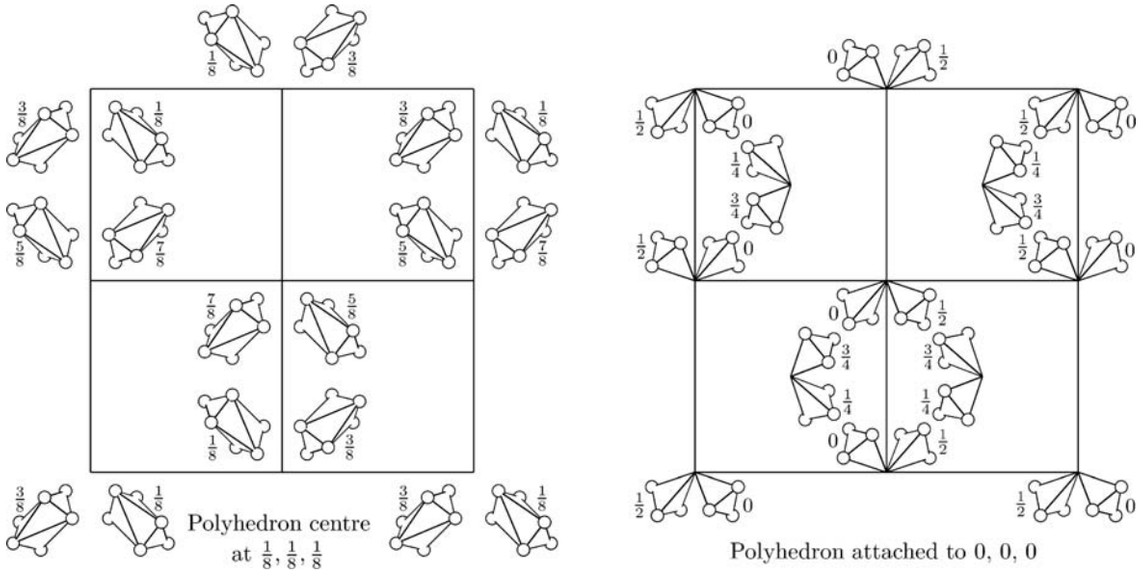

Figure 1.4.2.8
General-position diagrams for the space group $I4_132$ (214). Left: polyhedra (twisted trigonal antiprisms) with centres at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points (site-symmetry group .32). Right: polyhedra (sphenoids) attached to 0, 0, 0 and its equivalent points (site-symmetry group .3.).

some practice each of the diagrams can be generated from the other. In a number of texts, the two diagrams are considered as completely equivalent descriptions of the same space group. This statement is true for most of the space groups. However, there are a number of space groups for which the point configuration displayed on the general-position diagram has higher symmetry than the generating space group (Suescun & Nespolo, 2012; Müller, 2012). For example, consider the diagrams of the space group $P2$, No. 3 (unique axis b, cell choice 1) shown in Fig. 1.4.2.7. It is easy to recognise that, apart from the twofold rotations, the point configuration shown in the general-position diagram is symmetric with respect to a reflection through a plane containing the general-position points, and as a result the space group of the general-position configuration is of $P2/m$ type, and not of $P2$. There are a number of space groups for which the general-position diagram displays higher space-group symmetry, for example: $P1$, $P2_1$, $P4mm$, $P6$ *etc.* The analysis of the eigensymmetry groups of the general-position orbits results in a systematic procedure for the determination of such space groups: the general-position diagrams do not reflect the space-group symmetry correctly if the general-position orbits are *non-characteristic*, *i.e.* their eigensymmetry groups are supergroups of the space groups. (An introduction to terms like eigensymmetry groups, characteristic and non-characteristic orbits, and further discussion of space groups with non-characteristic general-position orbits are given in Section 1.4.4.4.)

(2) The graphical presentation of the general-position points of cubic groups is more difficult: three different parameters are required to specify the height of the points along the projection direction. To make the presentation clearer, the general-position points are grouped around points of higher site symmetry and represented in the form of polyhedra. For most of the space groups the initial general point is taken as 0.048, 0.12, 0.089, and the polyhedra are centred at 0, 0, 0 (and its equivalent points). Additional general-position diagrams are shown for space groups with special sites different from 0, 0, 0 that have site-symmetry groups of equal or higher order. Consider, for example, the two general-position diagrams of the space group $I4_132$ (214) shown in Fig. 1.4.2.8. The polyhedra of the left-hand diagram are centred at special points of highest site-symmetry, namely, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ and its equivalent points in the unit cell. The site-symmetry groups are of the type 32 leading to polyhedra in the form of *twisted trigonal antiprisms* (*cf.* Table 3.2.3.2). The polyhedra (sphenoids) of the right-hand diagram are attached to the origin 0, 0, 0 and its equivalent points in the unit cell, site-symmetry group of the type 3. The fractions attached to the polyhedra indicate the heights of the high-symmetry points along the projection direction (*cf.* Section 2.1.3.6 for further explanations of the diagrams).

Table 1.4.3.1
Sequence of generators for the crystal classes

The space-group generators differ from those listed here by their glide or screw components. The generator 1 is omitted, except for crystal class 1. The generators are represented by the corresponding Seitz symbols (*cf.* Tables 1.4.2.1–1.4.2.3). Following the conventions, the subscript of a symbol denotes the characteristic direction of that operation, where necessary. For example, the subscripts 001, 010, 110 *etc.* refer to the directions [001], [010], [110] *etc.* For mirror reflections m, the 'direction of m' refers to the normal of the mirror plane.

Hermann–Mauguin symbol of crystal class	Generators g_i (sequence left to right)
1	1
$\bar{1}$	$\bar{1}$
2	2
m	m
$2/m$	$2, \bar{1}$
222	$2_{001}, 2_{010}$
$mm2$	$2_{001}, m_{010}$
mmm	$2_{001}, 2_{010}, \bar{1}$
4	$2_{001}, 4^+_{001}$
$\bar{4}$	$2_{001}, \bar{4}^+_{001}$
$4/m$	$2_{001}, 4^+_{001}, \bar{1}$
422	$2_{001}, 4^+_{001}, 2_{010}$
$4mm$	$2_{001}, 4^+_{001}, m_{010}$
$\bar{4}2m$	$2_{001}, \bar{4}^+_{001}, 2_{010}$
$\bar{4}m2$	$2_{001}, \bar{4}^+_{001}, m_{010}$
$4/mmm$	$2_{001}, 4^+_{001}, 2_{010}, \bar{1}$
3	3^+_{001}
(rhombohedral coordinates	3^+_{111})
$\bar{3}$	$3^+_{001}, \bar{1}$
(rhombohedral coordinates	$3^+_{111}, \bar{1}$
321	$3^+_{001}, 2_{110}$
(rhombohedral coordinates	$3^+_{111}, 2_{\bar{1}01}$)
312	$3^+_{001}, 2_{1\bar{1}0}$
$3m1$	$3^+_{001}, m_{110}$
(rhombohedral coordinates	$3^+_{111}, m_{\bar{1}01}$)
$31m$	$3^+_{001}, m_{1\bar{1}0}$
$\bar{3}m1$	$3^+_{001}, 2_{110}, \bar{1}$
(rhombohedral coordinates	$3^+_{111}, 2_{\bar{1}01}, \bar{1}$)
$\bar{3}1m$	$3^+_{001}, 2_{1\bar{1}0}, \bar{1}$
6	$3^+_{001}, 2_{001}$
$\bar{6}$	$3^+_{001}, m_{001}$
$6/m$	$3^+_{001}, 2_{001}, \bar{1}$
622	$3^+_{001}, 2_{001}, 2_{110}$
$6mm$	$3^+_{001}, 2_{001}, m_{110}$
$\bar{6}m2$	$3^+_{001}, m_{001}, m_{110}$
$\bar{6}2m$	$3^+_{001}, m_{001}, 2_{110}$
$6/mmm$	$3^+_{001}, 2_{001}, 2_{110}, \bar{1}$
23	$2_{001}, 2_{010}, 3^+_{111}$
$m\bar{3}$	$2_{001}, 2_{010}, 3^+_{111}, \bar{1}$
432	$2_{001}, 2_{010}, 3^+_{111}, 2_{110}$
$\bar{4}3m$	$2_{001}, 2_{010}, 3^+_{111}, m_{1\bar{1}0}$
$m\bar{3}m$	$2_{001}, 2_{010}, 3^+_{111}, 2_{110}, \bar{1}$

1.4.3. Generation of space groups

By H. Wondratschek

In group theory, a *set of generators* of a group is a set of group elements such that each group element may be obtained as a finite ordered product of the generators. For space groups of one, two and three dimensions, generators may always be chosen and ordered in such a way that each symmetry operation W can be written as the product of powers of h generators g_j ($j = 1, 2, \ldots, h$). Thus,

$$W = g_h^{k_h} \cdot g_{h-1}^{k_{h-1}} \cdot \ldots \cdot g_p^{k_p} \cdot \ldots \cdot g_3^{k_3} \cdot g_2^{k_2} \cdot g_1,$$

where the powers k_j are positive or negative integers (including zero). The description of a group by means of generators has the advantage of compactness. For instance, the 48 symmetry operations in point group $m\bar{3}m$ can be described by two

Table 1.4.3.2
Generation of the space group $P6_122 \equiv D_6^2$ (178)

The entries in the second column designated by the numbers (1)–(12) correspond to the coordinate triplets of the general position of $P6_122$.

	Coordinate triplets	Symmetry operations
g_1	(1) x, y, z;	Identity I
g_2	$t(100)$	Generating translations
g_3	$t(010)$	
g_4	$t(001)$	
	The group $\mathcal{G}_4 \equiv \mathcal{T}$ of all translations of $P6_122$ has been generated	
g_5	(2) $\bar{y}, x-y, z+\frac{1}{3}$;	Threefold screw rotation
g_5^2	(3) $\bar{x}+y, \bar{x}, z+\frac{2}{3}$;	Threefold screw rotation
$g_5^3 = t(001)$:	Now the space group $\mathcal{G}_5 \equiv P3_1$ has been generated	
g_6	(4) $\bar{x}, \bar{y}, z+\frac{1}{2}$;	Twofold screw rotation
$g_6 * g_5$	(5) $y, \bar{x}+y, z+\frac{5}{6}$;	Sixfold screw rotation
$g_6 * g_5^2$	$x-y, x, z+\frac{7}{6} \sim$ (6) $x-y, x, z+\frac{1}{6}$;	Sixfold screw rotation
$g_6^2 = t(001)$:	Now the space group $\mathcal{G}_6 \equiv P6_1$ has been generated	
g_7	(7) $y, x, \bar{z}+\frac{1}{3}$;	Twofold rotation, direction of axis [110]
$g_7 * g_5$	(8) $x-y, \bar{y}, \bar{z}$;	Twofold rotation, axis [100]
$g_7 * g_5^2$	$\bar{x}, \bar{x}+y, \bar{z}-\frac{1}{3} \sim$ (9) $\bar{x}, \bar{x}+y, \bar{z}+\frac{2}{3}$;	Twofold rotation, axis [010]
$g_7 * g_6$	$\bar{y}, \bar{x}, \bar{z}-\frac{1}{6} \sim$ (10) $\bar{y}, \bar{x}, \bar{z}+\frac{5}{6}$;	Twofold rotation, axis $[1\bar{1}0]$
$g_7 * g_6 * g_5$	$\bar{x}+y, y, \bar{z}-\frac{1}{2} \sim$ (11) $\bar{x}+y, y, \bar{z}+\frac{1}{2}$;	Twofold rotation, axis [120]
$g_7 * g_6 * g_5^2$	$x, x-y, \bar{z}-\frac{5}{6} \sim$ (12) $x, x-y, \bar{z}+\frac{1}{6}$;	Twofold rotation, axis [210]
$g_7^2 = I$	$\mathcal{G}_7 \sim P6_122$	

generators. Different choices of generators are possible. For the space-group tables, generators and generating procedures have been chosen such as to make the entries in the blocks 'General position' (*cf.* Section 2.1.3.11) and 'Symmetry operations' (*cf.* Section 2.1.3.9) as transparent as possible. Space groups of the same crystal class are generated in the same way (see Table 1.4.3.1 for the sequences that have been chosen), and the aim has been to accentuate important subgroups of space groups as much as possible. Accordingly, a process of generation in the form of a *composition series* has been adopted, see Ledermann (1976). The generator g_1 is defined as the identity operation, represented by (1) x, y, z. The generators g_2, g_3, and g_4 are the translations with translation vectors **a**, **b** and **c**, respectively. Thus, the coefficients k_2, k_3 and k_4 may have any integral value. If centring translations exist, they are generated by translations g_5 (and g_6 in the case of an F lattice) with translation vectors **d** (and **e**). For a C lattice, for example, **d** is given by $\mathbf{d} = \frac{1}{2}(\mathbf{a}+\mathbf{b})$. The exponents k_5 (and k_6) are restricted to the following values:

Lattice letter A, B, C, I: $k_5 = 0$ or 1.

Lattice letter R (hexagonal axes): $k_5 = 0$, 1 or 2.

Lattice letter F: $k_5 = 0$ or 1; $k_6 = 0$ or 1.

As a consequence, any translation t of $\mathcal{G}$ with translation vector

$$\mathbf{t} = k_2\mathbf{a} + k_3\mathbf{b} + k_4\mathbf{c}\,(+k_5\mathbf{d} + k_6\mathbf{e})$$

can be obtained as a product

$$t = (g_6)^{k_6}.(g_5)^{k_5}.g_4^{k_4}.g_3^{k_3}.g_2^{k_2}.g_1,$$

where $k_2, \ldots, k_6$ are integers determined by t. The generators g_6 and g_5 are enclosed between parentheses because they are effective only in centred lattices.

The remaining generators generate those symmetry operations that are not translations. They are chosen in such a way that only terms g_j or g_j^2 occur. For further specific rules, see below.

The process of generating the entries of the space-group tables may be demonstrated by the example in Table 1.4.3.2, where $\mathcal{G}_j$ denotes the group generated by $g_1, g_2, \ldots, g_j$. For $j \geq 5$, the next generator g_{j+1} is introduced when $g_j^{k_j} \in \mathcal{G}_{j-1}$, because in this case no new symmetry operation would be generated by $g_j^{k_j}$. The generating process is terminated when there is no further generator. In the present example, g_7 completes the generation: $\mathcal{G}_7 \equiv P6_122$ (178).

1.4.3.1. Selected order for non-translational generators

For the non-translational generators, the following sequence has been adopted:

(*a*) In all centrosymmetric space groups, an inversion (if possible at the origin O) has been selected as the last generator.

(*b*) Rotations precede symmetry operations of the second kind. In crystal classes $\bar{4}2m$ and $\bar{4}m2$ and $\bar{6}2m$ and $\bar{6}m2$, as an exception, $\bar{4}$ and $\bar{6}$ are generated first in order to take into account the conventional choice of origin in the fixed points of $\bar{4}$ and $\bar{6}$.

(*c*) The non-translational generators of space groups with C, A, B, F, I or R symbols are those of the corresponding space group with a P symbol, if possible. For instance, the generators of $I2_12_12_1$ (24) are those of $P2_12_12_1$ (19) and the generators of *Ibca* (73) are those of *Pbca* (61), apart from the centring translations.

Exceptions: *I*4*cm* (108) and *I*4/*mcm* (140) are generated *via* *P*4*cc* (103) and *P*4/*mcc* (124), because *P*4*cm* and *P*4/*mcm* do not exist. In space groups with *d* glides (except $I\bar{4}2d$, No. 122) and also in $I4_1/a$ (88), the corresponding rotation subgroup has been generated first. The generators of this subgroup are the same as those of the corresponding space group with a lattice symbol *P*.

Example

$F4_1/d\bar{3}2/m$ (227):

$P4_132$ (213) $\longrightarrow$ $F4_132$ (210) $\longrightarrow$ $F4_1/d\bar{3}2/m$.

(*d*) In some cases, rule (*c*) could not be followed without breaking rule (*a*), *e.g.* in *Cmme* (67). In such cases, the generators are chosen to correspond to the Hermann–Mauguin symbol as far as possible. For instance, the generators (apart from centring) of *Cmme* and *Imma* (74) are

those of *Pmmb*, which is a non-standard setting of *Pmma* (51). (A combination of the generators of *Pmma* with the *C*- or *I*-centring translation results in non-standard settings of *Cmme* and *Imma*.)

For the space groups with lattice symbol *P*, the generation procedure has given the same triplets (except for their sequence) as in *IT* (1952). In non-*P* space groups, the triplets listed sometimes differ from those of *IT* (1952) by a centring translation.

1.4.4. General and special Wyckoff positions

By B. Souvignier

One of the first tasks in the analysis of crystal patterns is to determine the actual positions of the atoms. Since the full crystal pattern can be reconstructed from a single unit cell or even an asymmetric unit, it is clearly sufficient to focus on the atoms inside such a restricted volume. What one observes is that the atoms typically do not occupy arbitrary positions in the unit cell, but that they often lie on geometric elements, *e.g.* reflection planes or lines along rotation axes. It is therefore very useful to analyse the symmetry properties of the points in a unit cell in order to predict likely positions of atoms.

We note that in this chapter all statements and definitions refer to the usual three-dimensional space $\mathbb{E}^3$, but also can be formulated, *mutatis mutandis*, for plane groups acting on $\mathbb{E}^2$ and for higher-dimensional groups acting on n-dimensional space $\mathbb{E}^n$.

1.4.4.1. Crystallographic orbits

Since the operations of a space group provide symmetries of a crystal pattern, two points X and Y that are mapped onto each other by a space-group operation are regarded as being *geometrically equivalent*. Starting from a point $X \in \mathbb{E}^3$, infinitely many points Y equivalent to X are obtained by applying all space-group operations $g = (\boldsymbol{W}, \boldsymbol{w})$ to X: $Y = g(X) = (\boldsymbol{W}, \boldsymbol{w})X = (\boldsymbol{W}X + \boldsymbol{w})$.

Definition

For a space group $\mathcal{G}$ acting on the three-dimensional space $\mathbb{E}^3$, the (infinite) set

$$\mathcal{O} = \mathcal{G}(X) := \{g(X) | g \in \mathcal{G}\}$$

is called the *orbit of X under* $\mathcal{G}$.

The orbit of X is the smallest subset of $\mathbb{E}^3$ that contains X and is closed under the action of $\mathcal{G}$. It is also called a *crystallographic orbit*.

Every point in direct space $\mathbb{E}^3$ belongs to precisely one orbit under $\mathcal{G}$ and thus the orbits of $\mathcal{G}$ partition the direct space into disjoint subsets. It is clear that an orbit is completely determined by its points in the unit cell, since translating the unit cell by the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ entirely covers $\mathbb{E}^3$.

It may happen that two different symmetry operations g and h in $\mathcal{G}$ map X to the same point. Since $g(X) = h(X)$ implies that $h^{-1}g(X) = X$, the point X is fixed by the nontrivial operation $h^{-1}g$ in $\mathcal{G}$.

Definition

The subgroup $\mathcal{S}_X = \mathcal{S}_{\mathcal{G}}(X) := \{g \in \mathcal{G} | g(X) = X\}$ of symmetry operations from $\mathcal{G}$ that fix X is called the *site-symmetry group of X in* $\mathcal{G}$.

Since translations, glide reflections and screw rotations fix no point in $\mathbb{E}^3$, a site-symmetry group $\mathcal{S}_X$ never contains operations of these types and thus consists only of reflections, rotations, inversions and rotoinversions. Because of the absence of translations, $\mathcal{S}_X$ contains at most one operation from a coset $\mathcal{T}g$ relative to the translation subgroup $\mathcal{T}$ of $\mathcal{G}$, since otherwise the quotient of two such operations tg and $t'g$ would be the nontrivial translation $tgg^{-1}t'^{-1} = tt'^{-1}$ (see Chapter 1.3 for a discussion of coset decompositions). In particular, the operations in $\mathcal{S}_X$ all have different linear parts and because these linear parts form a subgroup of the point group $\mathcal{P}$ of $\mathcal{G}$, the order of the site-symmetry group $\mathcal{S}_X$ is a divisor of the order of the point group of $\mathcal{G}$.

The site-symmetry group of a point X is thus a finite subgroup of the space group $\mathcal{G}$, a subgroup which is isomorphic to a subgroup of the point group $\mathcal{P}$ of $\mathcal{G}$.

Example

For a space group $\mathcal{G}$ of type $P\bar{1}$, the site-symmetry group of the origin $X = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ is clearly generated by the inversion in the origin: $\{\bar{1}|0\}(X) = X$. On the other hand, the point $Y = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$ is fixed by the inversion in Y, *i.e.*

$$\{\bar{1}|1,0,1\}(Y) = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix} = Y.$$

The symmetry operation $\{\bar{1}|1,0,1\}$ also belongs to $\mathcal{G}$ and generates the site-symmetry group of Y. The site-symmetry groups $\mathcal{S}_X = \{\{1|0\}, \{\bar{1}|0\}\}$ of X and $\mathcal{S}_Y = \{\{1|0\}, \{\bar{1}|1,0,1\}\}$ of Y are thus different subgroups of order 2 of $\mathcal{G}$ which are isomorphic to the point group of $\mathcal{G}$ (which is generated by $\bar{1}$).

The order $|\mathcal{S}_X|$ of the site-symmetry group $\mathcal{S}_X$ is closely related to the number of points in the orbit of X that lie in the unit cell. An application of the orbit–stabilizer theorem (see Section 1.1.7) yields the crucial observation that each point $Y = g(X)$ in the orbit of X under $\mathcal{G}$ is obtained precisely $|\mathcal{S}_X|$ times as an orbit point: for each $h \in \mathcal{S}_X$ one has $gh(X) = g(X) = Y$ and conversely $g'(X) = g(X)$ implies that $g^{-1}g' = h \in \mathcal{S}_X$ and thus $g' = gh$ for an operation h in $\mathcal{S}_X$.

Assuming first that we are dealing with a space group $\mathcal{G}$ described by a *primitive* lattice, each coset of $\mathcal{G}$ relative to the translation subgroup $\mathcal{T}$ contains precisely one operation g such that $g(X)$ lies in the primitive unit cell. Since the number of cosets equals the order $|\mathcal{P}|$ of the point group $\mathcal{P}$ of $\mathcal{G}$ and since each orbit point is obtained $|\mathcal{S}_X|$ times, it follows that the number of orbit points in the unit cell is $|\mathcal{P}|/|\mathcal{S}_X|$.

If we deal with a space group with a centred unit cell, the above result has to be modified slightly. If there are $k - 1$ centring vectors, the lattice spanned by the conventional basis is a sublattice of index k in the full translation lattice. The conventional cell therefore is built up from k primitive unit cells (spanned by a primitive lattice basis) and thus in particular contains k times as many points as the primitive cell (see Chapter 1.3 for a detailed discussion of conventional and primitive bases and cells).

Proposition

Let $\mathcal{G}$ be a space group with point group $\mathcal{P}$ and let $\mathcal{S}_X$ be the site-symmetry group of a point X in $\mathbb{E}^3$. Then the number of orbit points of the orbit of X which lie in a conventional cell for $\mathcal{G}$ is equal to the product $k \times |\mathcal{P}|/|\mathcal{S}_X|$, where k is the volume of the conventional cell divided by the volume of a primitive unit cell.

1.4.4.2. Wyckoff positions

As already mentioned, one of the first issues in the analysis of crystal structures is the determination of the actual atom positions. Energetically favourable configurations in inorganic compounds are often achieved when the atoms occupy positions that have a nontrivial site-symmetry group. This suggests that one should classify the points in $\mathbb{E}^3$ into equivalence classes according to their site-symmetry groups.

Definition

A point $X \in \mathbb{E}^3$ is called a point in a *general position* for the space group $\mathcal{G}$ if its site-symmetry group contains only the identity element of $\mathcal{G}$. Otherwise, X is called a point in a *special position*.

The distinctive feature of a point in a general position is that the points in its orbit are in one-to-one correspondence with the symmetry operations of the group $\mathcal{G}$ by associating the orbit point $g(X)$ with the group operation g. For different group elements g and g', the orbit points $g(X)$ and $g'(X)$ must be different, since otherwise $g^{-1}g'$ would be a non-trivial operation in the site-symmetry group of X. Therefore, the entries listed in the space-group tables for the general positions can not only be interpreted as a shorthand notation for the symmetry operations in $\mathcal{G}$ (as seen in Section 1.4.2.3), but also as coordinates of the points in the orbit of a point X in a general position with coordinates x, y, z (up to translations).

Whereas points in general positions exist for every space group, not every space group has points in a special position. Such groups are called *fixed-point-free space groups* or *Bieberbach groups* and are precisely those groups that may contain glide reflections or screw rotations, but no proper reflections, rotations, inversions and rotoinversions.

Example

The group $\mathcal{G}$ of type $Pna2_1$ (33) has a point group of order 4 and representatives for the non-trivial cosets relative to the translation subgroup are the twofold screw rotation $\bar{x}, \bar{y}, z + \frac{1}{2}$, the a glide $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z$ and the n glide $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$. No operation in the coset of the twofold screw rotation can have a fixed point, since such an operation maps the z component to $z + \frac{1}{2} + t_z$ for an integer t_z, and this is never equal to z. The same argument applies to the x component of the a glide and to the y component of the n glide, hence this group contains no operation with a fixed point (apart from the identity element) and is thus a fixed-point-free space group.

The distinction into general and special positions is of course very coarse. In a finer classification, it is certainly desirable that two points in the same orbit under the space group belong to the same class, since they are symmetry equivalent. Such points have *conjugate* site-symmetry groups (*cf.* the orbit–stabilizer theorem in Section 1.1.7).

Lemma

Let X and Y be points in the same orbit of a space group $\mathcal{G}$ and let $g \in \mathcal{G}$ such that $g(X) = Y$. Then the site-symmetry groups of X and Y are conjugate by the operation mapping X to Y, *i.e.* one has $\mathcal{S}_Y = g \cdot \mathcal{S}_X \cdot g^{-1}$.

The classification motivated by the conjugacy relation between the site-symmetry groups of points in the same orbit is the classification into *Wyckoff positions*.

Definition

Two points X and Y in $\mathbb{E}^3$ belong to the same *Wyckoff position* with respect to $\mathcal{G}$ if their site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of $\mathcal{G}$.

In particular, the Wyckoff position containing a point X also contains the full orbit $\mathcal{G}(X)$ of X under $\mathcal{G}$.

Remark: It is built into the definition of Wyckoff positions that points that are related by a symmetry operation of $\mathcal{G}$ belong to the same Wyckoff position. However, a single site-symmetry group may have more than one fixed point, *e.g.* points on the same rotation axis or in the same reflection plane. These points are in general not symmetry related but, having identical site-symmetry groups, clearly belong to the same Wyckoff position. This situation can be analyzed more explicitly:

Let $\mathcal{S}_X$ be the site-symmetry group of the point X and assume that Y is another point with the same site-symmetry group $\mathcal{S}_Y = \mathcal{S}_X$. Choosing a coordinate system with origin X, the operations in $\mathcal{S}_X$ all have translational part equal to zero and are thus matrix–column pairs of the form $(\boldsymbol{W}, \boldsymbol{o})$. In particular, these operations are *linear* operations, and since both points X and Y are fixed by all operations in $\mathcal{S}_X$, the vector $\mathbf{v} = Y - X$ is also fixed by the linear operations $(\boldsymbol{W}, \boldsymbol{o})$ in $\mathcal{S}_X$. But with the vector $\mathbf{v}$ each scaling $c \cdot \mathbf{v}$ of $\mathbf{v}$ is fixed as well, and therefore all the points on the line through X and Y are fixed by the operations in $\mathcal{S}_X$. This shows that the Wyckoff position of X is a union of infinitely many orbits if $\mathcal{S}_X$ has more than one fixed point.

Lemma

Let $\mathcal{S}_X$ be the site-symmetry group of X in $\mathcal{G}$:

(i) The points belonging to the same Wyckoff position as X are precisely the points in the orbit of X under $\mathcal{G}$ if and only if X is the only point fixed by all operations in $\mathcal{S}_X$. In this case the coordinates of a point belonging to this Wyckoff position have fixed values not depending on a parameter.

(ii) If Y is a further point fixed by all operations in $\mathcal{S}_X$ but there is no fixed point of $\mathcal{S}_X$ outside the line through X and Y, then all the points on the line through X and Y are fixed by $\mathcal{S}_X$. The Wyckoff position of X is then the union of the orbits of points on this line (with the exception of a possibly empty discrete subset of points which have a larger site-symmetry group). In this case the coordinates of a point belonging to this Wyckoff position have values depending on a single variable parameter.

(iii) If Y and Z are points fixed by all operations in $\mathcal{S}_X$ such that X, Y, Z do not lie on a line, then all the points on the plane through X, Y and Z are fixed by $\mathcal{S}_X$. The Wyckoff position of X is then the union of the orbits of points in this plane with the exception of a (possibly empty) discrete subset of lines or points which have a larger site-symmetry group. In this case the coordinates of a point belonging to this Wyckoff position have values depending on two variable parameters.

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			
8	*d* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
		(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$

Figure 1.4.4.1
General-position block as given in the space-group tables for space group *P*4*bm* (100).

(iv) Only the points belonging to the general position depend on three variable parameters.

The space-group tables of Chapter 2.3 contain the following information about the Wyckoff positions of a space group $\mathcal{G}$:

Multiplicity: The Wyckoff multiplicity is the number of points in an orbit for this Wyckoff position which lie in the conventional cell. For a group with a primitive unit cell, the multiplicity for the general position equals the order of the point group of $\mathcal{G}$, while for a centred cell this is multiplied by the quotient of the volumes of the conventional cell and a primitive unit cell.

The quotient of the multiplicity for the general position by that of a special position gives the order of the site-symmetry group of the special position.

Wyckoff letter: Each Wyckoff position is labelled by a letter in alphabetical order, starting with '*a*' for a position with site-symmetry group of maximal order and ending with the highest letter (corresponding to the number of different Wyckoff positions) for the general position.

It is common to specify a Wyckoff position by its multiplicity and Wyckoff letter, *e.g.* by 4*a* for a position with multiplicity 4 and letter *a*.

Site symmetry: The point group isomorphic to the site-symmetry group is indicated by an *oriented symbol*, which is a variation of the Hermann–Mauguin point-group symbol that provides information about the orientation of the symmetry elements. The constituents of the oriented symbol are ordered according to the symmetry directions of the corresponding crystal lattice (primary, secondary and tertiary). A symmetry operation in the site-symmetry group gives rise to a symbol in the position corresponding to the direction of its geometric element. Directions for which no symmetry operation contributes to the site-symmetry group are represented by a dot in the oriented symbol.

Coordinates: Under this heading, the coordinates of the points in an orbit belonging to the Wyckoff position are given, possibly depending on one or two variable parameters (three for the general position). The points given represent the orbit up to translations from the full translational subgroup. For a space group with a centred lattice, centring vectors which are coset representatives for the translation lattice relative to the lattice spanned by the conventional basis are given at the top of the table. To obtain representatives of the orbit up to translations from the lattice spanned by the conventional basis, these centring vectors have to be added to each of the given points.

As already mentioned, the coordinates given for the general position can also be interpreted as a compact notation for the symmetry operations, specified up to translations.

The entries in the last column, the *reflection conditions*, are discussed in detail in Chapter 1.6. This column lists the conditions for the reflection indices *hkl* for which the corresponding structure factor is not systematically zero.

Examples

(1) Let $\mathcal{G}$ be the space group of type *Pbca* (61) generated by the twofold screw rotations $\{2_{001}|\frac{1}{2},0,\frac{1}{2}\}$: $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ and $\{2_{010}|0,\frac{1}{2},\frac{1}{2}\}$: $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$, the inversion $\{\bar{1}|0\}$: $\bar{x},\bar{y},\bar{z}$ and the translations $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$.
Applying the eight coset representatives of $\mathcal{G}$ with respect to the translation subgroup, the points in the orbit of the origin $X_1 = \begin{pmatrix}0\\0\\0\end{pmatrix}$ that lie in the unit cell are found to be X_1, $X_2 = \begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$, $X_3 = \begin{pmatrix}0\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$ and $X_4 = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix}$, and the Wyckoff position to which X_1 belongs has multiplicity 4 and is labelled 4*a*.
Since the point group $\mathcal{P}$ of $\mathcal{G}$ has order 8, the site-symmetry group $\mathcal{S}_{X_1}$ has order 8/4 = 2. The inversion in the origin X_1 obviously fixes X_1, hence $\mathcal{S}_{X_1} = \{\{1|0\},\{\bar{1}|0\}\}$. The oriented symbol for the site symmetry is $\overline{1}$, indicating that the site-symmetry group is generated by an inversion.
The points X_2, X_3 and X_4 belong to the same Wyckoff position as X_1, since they lie in the orbit of X_1 and thus have conjugate site-symmetry groups.
The point $Y_1 = \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix}$ also has an orbit with 4 points in the unit cell, namely Y_1, $Y_2 = \begin{pmatrix}\frac{1}{2}\\0\\0\end{pmatrix}$, $Y_3 = \begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$ and $Y_4 = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}$. These points therefore belong to a common Wyckoff position, namely position 4*b*. Moreover, the site-symmetry group of Y_1 is also generated by an inversion, namely the inversion $\{\bar{1}|0,0,1\}$: $\bar{x},\bar{y},\bar{z}+1$ located at Y_1 and is thus denoted by the oriented symbol $\overline{1}$.
The points X_1 and Y_1 do not belong to the same Wyckoff position, because an operation $(\boldsymbol{W},\boldsymbol{w})$ in $\mathcal{G}$ conjugates the inversion $\{\bar{1}|0,0,0\}$ in the origin to an inversion in $\boldsymbol{w}$. Since the translational parts of the operations in $\mathcal{G}$ are (up to integers) $(0,0,0)$, $(\frac{1}{2},\frac{1}{2},0)$, $(\frac{1}{2},0,\frac{1}{2})$ and $(0,\frac{1}{2},\frac{1}{2})$, an inversion in $Y_1 = \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix}$ can not be obtained by conjugation with operations from $\mathcal{G}$.

(2) Let $\mathcal{G}$ be the space group of type *P*4*bm* (100) generated by the fourfold rotation $\{4^+|0\}$: $\bar{y},x,z$, the glide reflection (of *b* type) $\{m_{100}|\frac{1}{2},\frac{1}{2},0\}$: $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$ and the translations $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$. The general-position coordinate triplets are shown in Fig. 1.4.4.1
From this information, the coordinates for the orbit of a specific point X in a special position can be derived by simply inserting the coordinates of X into the general-

position coordinates, normalizing to values between 0 and 1 (by adding ± 1 if required) and eliminating duplicates.

For example, for the point $X = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{4} \end{pmatrix}$ in Wyckoff position 2*b* one obtains X and $Y = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}$ as the points in the orbit of X that lie in the unit cell. Since the point group $\mathcal{P}$ of $\mathcal{G}$ has order 8, the site-symmetry group $\mathcal{S}_X$ is a group of order 8/2 = 4. Its four operations are

Coordinate triplet	Description
x, y, z	Identity operation
$\bar{x}+1, \bar{y}, z$	Twofold rotation with axis $\frac{1}{2}, 0, z$
$\bar{y}+\frac{1}{2}, \bar{x}+\frac{1}{2}, z$	Reflection with plane $x+\frac{1}{2}, -x, z$
$y+\frac{1}{2}, x-\frac{1}{2}, z$	Reflection with plane $x+\frac{1}{2}, x, z$

The corresponding oriented symbol for the site-symmetry is 2.*mm*, indicating that the site-symmetry group contains a twofold rotation along a primary lattice direction, no symmetry operations along the secondary directions and two reflections along tertiary directions.

Since X and Y lie in the same orbit, they clearly belong to the same Wyckoff position. But every point $X' = \begin{pmatrix} \frac{1}{2} \\ 0 \\ z \end{pmatrix}$ with $0 \le z < 1$ has the same site-symmetry group as X and therefore also belongs to the same Wyckoff position as X. Inserting the coordinates of X' in the general-position coordinates, one obtains $Y' = \begin{pmatrix} 0 \\ \frac{1}{2} \\ z \end{pmatrix}$ as the only other point in the orbit of X' that lies in the unit cell. Clearly, Y' has the same site-symmetry group as Y. The Wyckoff position 2*b* to which X belongs therefore consists of the union of the orbits of the points $X' = \begin{pmatrix} \frac{1}{2} \\ 0 \\ z \end{pmatrix}$ with $0 \le z < 1$.

In the space-group diagram in Fig. 1.4.4.2, the points belonging to Wyckoff position 2*b* can be identified as the points on the intersection of a twofold rotation axis directed along [001] and two reflection planes normal to the square diagonals and crossing the centres of the sides bordering the unit cell. It is clear that for every value of z, the four intersection points in the unit cell lie in one orbit under the fourfold rotation located in the centre of the displayed cell.

Applying the same procedure to a point $X = \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}$ in Wyckoff position 2*a*, the points in the orbit that lie in the unit cell are seen to be X and $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ z \end{pmatrix}$. The site-symmetry group $\mathcal{S}_X$ is again of order 4 and since the fourfold rotation $\{4^+|0\}$ fixes X, $\mathcal{S}_X$ is the cyclic group of order 4 generated by this fourfold rotation. The oriented symbol for this site-symmetry group is 4.. and the corresponding points can easily be identified in the space-group diagram in Fig. 1.4.4.2 by the symbol for a fourfold rotation.

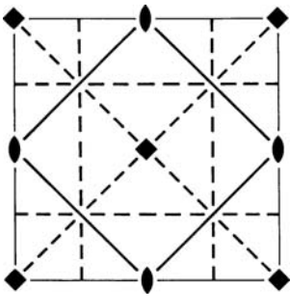

Figure 1.4.4.2
Symmetry-element diagram for the space group *P*4*bm* (100) for the orthogonal projection along [001].

Since a point in a special position has to lie on the geometric element of a reflection, rotation or inversion, the special positions can in principle be read off from the space-group diagrams. In the present example, we have dealt with the positions fixed by twofold or fourfold rotations, and from the diagram in Fig. 1.4.4.2 one sees that the only remaining case is that of points on reflection planes, indicated by the solid lines. A point on such a reflection plane is $X = \begin{pmatrix} x \\ x+\frac{1}{2} \\ z \end{pmatrix}$ and by inserting these coordinates into the general-position coordinates one obtains the points $\bar{x}, \bar{x}+\frac{1}{2}, z$, $\bar{x}+\frac{1}{2}, x, z$ and $x+\frac{1}{2}, \bar{x}, z$ as the other points in the orbit of X (up to translations). Here, the site-symmetry group $\mathcal{S}_X$ is of order 2, it is generated by the reflection $\{m_{1\bar{1}0}|-\frac{1}{2}, \frac{1}{2}, 0\}$: $y-\frac{1}{2}, x+\frac{1}{2}, z$ having the plane $x, x+\frac{1}{2}, z$ as geometric element. The oriented symbol of $\mathcal{S}_X$ is ..*m*, since the reflection is along a tertiary direction.

1.4.4.3. Wyckoff sets

Points belonging to the same Wyckoff position have conjugate site-symmetry groups and thus in particular all those points are collected together that lie in one orbit under the space group $\mathcal{G}$. However, in addition, points that are not symmetry-related by a symmetry operation in $\mathcal{G}$ may still play geometrically equivalent roles, *e.g.* as intersections of rotation axes with certain reflection planes.

Example

In the conventional setting, the fourfold axes of a space group $\mathcal{G}$ of type *P*4 (75) intersect the *ab* plane in the points $u_1, u_2, 0$ and $u_1+\frac{1}{2}, u_2+\frac{1}{2}, 0$ for integers u_1, u_2, as can be seen from the space-group diagram in Fig. 1.4.4.3.

The points $u_1, u_2, 0$ lie in one orbit under the translation subgroup of $\mathcal{G}$, and thus belong to the same Wyckoff position, labelled 1*a*. For the same reason, the points $u_1+\frac{1}{2}, u_2+\frac{1}{2}, 0$ belong to a single Wyckoff position, namely to position 1*b*. The points $X = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ and $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ do not belong to the same Wyckoff position, because the site-symmetry group $\mathcal{S}_X$ is generated by the fourfold rotation 4_{001} and conjugating this by an operation $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$ results in a fourfold rotation with axis parallel to the *c* axis and running through $\boldsymbol{w}$. But since the translation parts of all operations in $\mathcal{G}$ are integral, such an axis

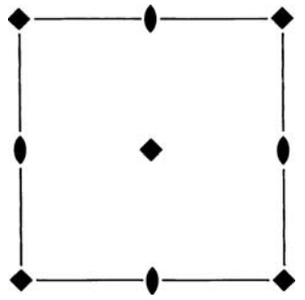

Figure 1.4.4.3
Symmetry-element diagram for the space group $P4$ (75) for the orthogonal projection along [001].

can not contain $Y = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and thus $\mathcal{S}_X$ and $\mathcal{S}_Y$ are not conjugate in $\mathcal{G}$.

However, the translation by $(\frac{1}{2}, \frac{1}{2}, 0)$ conjugates $\mathcal{S}_X$ to $\mathcal{S}_Y$, while fixing the group $\mathcal{G}$ as a whole. This shows that there is an ambiguity in choosing the origin either at 0, 0, 0 or $\frac{1}{2}, \frac{1}{2}, 0$, since these points are geometrically indistinguishable (both being intersections of a fourfold axis with the *ab* plane).

The ambiguity in the origin choice in the above example can be explained by the *affine normalizer* of the space group $\mathcal{G}$ (see Section 1.1.8 for a general introduction to normalizers). The full group $\mathcal{A}$ of affine mappings acts *via* conjugation on the set of space groups and the space groups of the same affine type are obtained as the orbit of a single group of that type under $\mathcal{A}$.

Definition

The group $\mathcal{N}$ of affine mappings $n \in \mathcal{A}$ that fix a space group $\mathcal{G}$ under conjugation is called the *affine normalizer* of $\mathcal{G}$, *i.e.*

$$\mathcal{N} = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = \{n \in \mathcal{A} | n\mathcal{G}n^{-1} = \mathcal{G}\}.$$

The affine normalizer is the largest subgroup of $\mathcal{A}$ such that $\mathcal{G}$ is a normal subgroup of $\mathcal{N}$.

Conjugation by operations of the affine normalizer results in a permutation of the operations of $\mathcal{G}$, *i.e.* in a relabelling without changing their geometric properties. The additional translations contained in the affine normalizer can in fact be derived from the space-group diagrams, because shifting the origin by such a translation results in precisely the same diagram. More generally, an element of the affine normalizer can be interpreted as a change of the coordinate system that does not alter the space-group diagrams.

A more thorough description of the affine normalizers of space groups is given in Chapter 3.5, where tables with the affine normalizers are also provided.

Since the affine normalizer of a space group $\mathcal{G}$ is in general a group containing $\mathcal{G}$ as a proper subgroup, it is possible that subgroups of $\mathcal{G}$ that are not conjugate by any operation of $\mathcal{G}$ may be conjugate by an operation in the affine normalizer. As a consequence, the site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ of two points X and Y belonging to different Wyckoff positions of $\mathcal{G}$ may be conjugate under the affine normalizer of $\mathcal{G}$. This reveals that the points X and Y are in fact geometrically equivalent, since they fall into the same orbit under the affine normalizer of $\mathcal{G}$. Joining the equivalence classes of these points into a single class results in a coarser classification with larger classes, which are called *Wyckoff sets*.

Definition

Two points X and Y belong to the same *Wyckoff set* if their site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of the affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ of $\mathcal{G}$.

In particular, the Wyckoff set containing a point X also contains the full orbit of X under the affine normalizer of $\mathcal{G}$.

Example

Let $\mathcal{G}$ be the space group of type $P222_1$ (17) generated by the translations of an orthorhombic lattice, the twofold rotation $\{2_{100}|0\}$: $x, \bar{y}, \bar{z}$ and the twofold screw rotation $\{2_{001}|0, 0, \frac{1}{2}\}$: $\bar{x}, \bar{y}, z + \frac{1}{2}$. Note that the composition of these two elements is the twofold rotation with the line $0, y, \frac{1}{4}$ as its geometric element. The group $\mathcal{G}$ has four different Wyckoff positions with a site-symmetry group generated by a twofold rotation; representatives of these Wyckoff positions are the points $X_1 = \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix}$ (Wyckoff position $2a$, site-symmetry symbol 2..), $X_2 = \begin{pmatrix} x \\ \frac{1}{2} \\ 0 \end{pmatrix}$ (position $2b$, symbol 2..), $Y_1 = \begin{pmatrix} 0 \\ y \\ \frac{1}{4} \end{pmatrix}$ (position $2c$, symbol .2.) and $Y_2 = \begin{pmatrix} \frac{1}{2} \\ y \\ \frac{1}{4} \end{pmatrix}$ (position $2d$, symbol .2.).

From the tables of affine normalizers in Chapter 3.5, but also by a careful analysis of the space-group diagrams in Fig. 1.4.4.4, one deduces that the affine normalizer of $\mathcal{G}$ contains the additional translations $t(\frac{1}{2}, 0, 0)$, $t(0, \frac{1}{2}, 0)$ and $t(0, 0, \frac{1}{2})$, since all the diagrams are invariant by a shift of $\frac{1}{2}$ along any of the coordinate axes. Moreover, the symmetry operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$: $y, x, z + \frac{1}{4}$ which interchanges the a and b axes and shifts the origin by $\frac{1}{4}$ along the c axis belongs to the affine

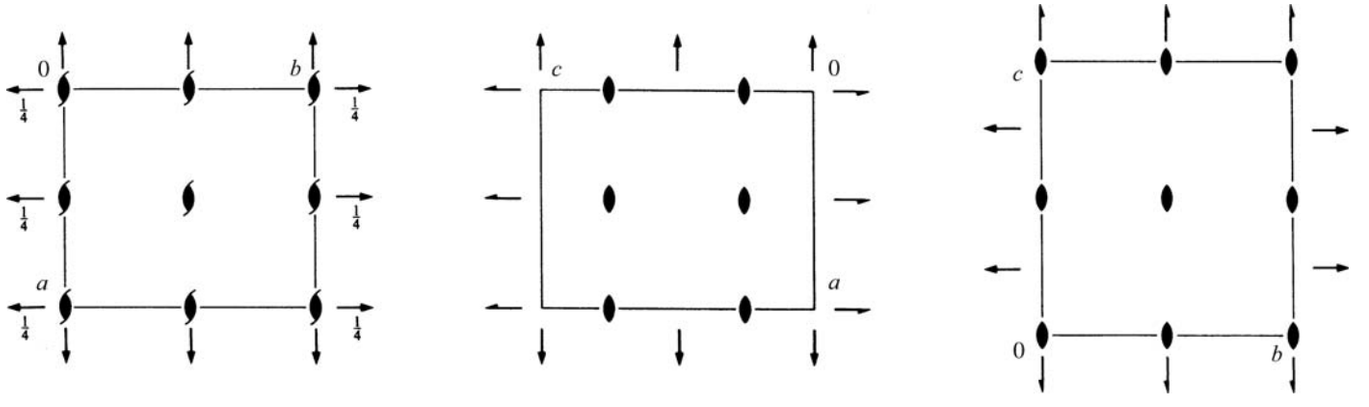

Figure 1.4.4.4
Symmetry-element diagrams for the space group $P222_1$ (17) for orthogonal projections along [001], [010], [100] (left to right).

normalizer, because it precisely interchanges the twofold rotations around axes parallel to the a and to the b axes. The translation $t(0, \frac{1}{2}, 0)$ maps X_1 to X_2, and hence X_1 and X_2 have site-symmetry groups which are conjugate under the affine normalizer of $\mathcal{G}$ and thus belong to the same Wyckoff set. Analogously, Y_1 and Y_2 belong to the same Wyckoff set, because $t(\frac{1}{2}, 0, 0)$ maps Y_1 to Y_2. Finally, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ found in the affine normalizer maps X_1 to Y_1. This shows that the points of all four Wyckoff positions actually belong to the same Wyckoff set.

Geometrically, the positions in this Wyckoff set can be described as those points that lie on a twofold rotation axis.

The assignments of Wyckoff positions of plane and space groups to Wyckoff sets are discussed and tabulated in Chapter 3.4.

Remark: The previous example deserves some further discussion. The group $\mathcal{G}$ of type $P222_1$ belongs to the orthorhombic crystal family, and the conventional unit cell is spanned by three basis vectors **a**, **b**, **c** with lengths a, b, c and right angles between each pair of basis vectors. Unless the parameters a and b are equal because of some metric specialization, the operation $\{m_{1\bar{1}0}|0, 0, \frac{1}{4}\}$ of the affine normalizer is not an isometry but changes lengths. If it is desired that the metric properties are preserved, the full affine normalizer cannot be taken into account, but only the subgroup that consists of isometries. This subgroup is called the *Euclidean normalizer* of $\mathcal{G}$. (A detailed discussion of Euclidean normalizers of space groups and their tabulation are given in Chapter 3.5.)

Taking conjugacy of the site-symmetry groups under the Euclidean normalizer as a condition results in a notion of equivalence which lies between that of Wyckoff positions and Wyckoff sets. In the above example, the four Wyckoff positions would be merged into two classes represented by X_1 and Y_1, but X_1 and Y_1 would not be regarded as equivalent, since they are not related by an operation of the Euclidean normalizer.

It turns out, however, that in many cases this intermediate classification coincides with the Wyckoff sets, because points belonging to different Wyckoff positions are often related to each other by a translation contained in the affine normalizer. Since translations are always isometries, the translations contained in the affine normalizer always belong to the Euclidean normalizer as well.

1.4.4.4. Eigensymmetry groups and non-characteristic orbits

A crystallographic orbit $\mathcal{O}$ has been defined as the set of points $g(X)$ obtained by applying all operations of some space group $\mathcal{G}$ to a point $X \in \mathbb{E}^3$. From that it is clear that the set $\mathcal{O}$ is invariant as a whole under the action of operations in $\mathcal{G}$, since for some point $Y = g(X)$ in the orbit and $h \in \mathcal{G}$ one has $h(Y) = (hg)(X)$, which is again contained in $\mathcal{O}$ because hg belongs to $\mathcal{G}$. However, it is possible that the orbit $\mathcal{O}$ is also invariant under some isometries of $\mathbb{E}^3$ that are not contained in $\mathcal{G}$. Since the composition of two such isometries still keeps the orbit invariant, the set of all isometries leaving $\mathcal{O}$ invariant forms a group which contains $\mathcal{G}$ as a subgroup.

Definition

Let $\mathcal{O} = \{g(X)|g \in \mathcal{G}\}$ be the orbit of a point $X \in \mathbb{E}^3$ under a space group $\mathcal{G}$. Then the group $\mathscr{E}$ of isometries of $\mathbb{E}^3$ which leave $\mathcal{O}$ invariant as a whole is called the *eigensymmetry group* of $\mathcal{O}$.

Since the orbit is a discrete set, the eigensymmetry group has to be a space group itself. One distinguishes the following cases:

(i) The eigensymmetry group $\mathscr{E}$ equals the group $\mathcal{G}$ by which the orbit was generated. In this case the orbit is called a *characteristic orbit* of $\mathcal{G}$.

(ii) The eigensymmetry group $\mathscr{E}$ contains $\mathcal{G}$ as a proper subgroup. Then the orbit is called a *non-characteristic orbit*.

(iii) If the eigensymmetry group $\mathscr{E}$ contains translations that are not contained in $\mathcal{G}$, *i.e.* if $\mathcal{T}_\mathcal{G}$ is a proper subgroup of $\mathcal{T}_\mathscr{E}$, the orbit is called an *extraordinary orbit*. Of course, extraordinary orbits are a special kind of non-characteristic orbits.

Non-characteristic orbits are closely related to the concept of *lattice complexes*, which are discussed in Chapter 3.4. An extensive listing of non-characteristic orbits of space groups can be found in Engel *et al.* (1984).

The fact that an orbit of a space group has a larger eigensymmetry group is an important example of a pair of groups that are in a group–subgroup relation. Knowledge of subgroups and supergroups of a given space group play a crucial role in the analysis of phase transitions, for example, and are discussed in detail in Chapter 1.7.

The occurrence of non-characteristic orbits does not require the point X to be chosen at a special position. Even the general position of a space group $\mathcal{G}$ may give rise to a non-characteristic orbit. Moreover, special values of the coordinates of the general position may give rise to additional eigensymmetries without the position becoming a special position. Conversely, the orbit of a point at a special position need not be non-characteristic.

Example

We compare space groups of types $P4_1$ (76) and $P4_2$ (77). For a space group of type $P4_1$, the general position with generic coordinates x, y, z gives rise to a characteristic orbit, whereas the general-position orbit for a space group of type $P4_2$ consists of the points $X_1 = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$, $X_2 = \begin{pmatrix} \overline{x} \\ \overline{y} \\ z \end{pmatrix}$, $X_3 = \begin{pmatrix} \overline{y} \\ x \\ z + \frac{1}{2} \end{pmatrix}$ and $X_4 = \begin{pmatrix} y \\ \overline{x} \\ z + \frac{1}{2} \end{pmatrix}$. An inversion $\{\overline{1}|0, 0, 2z\}$ in $0, 0, z$ interchanges X_1 and X_2, and maps X_3 to $y, \overline{x}, z - \frac{1}{2}$, which is clearly equivalent to X_4 under a translation. This shows that the general-position orbit for a space group of type $P4_2$ is a non-characteristic orbit, and the eigensymmetry group of this orbit is of type $P4_2/m$ (84), where the origin has to be shifted to the inversion point $0, 0, z$ to obtain the conventional setting. Since the unit cell and the orbit are unchanged, but the point group of $P4_2$ is a subgroup of index 2 in the point group of $P4_2/m$, the orbit points must belong to a special position for $P4_2/m$, namely the position labelled $4j$. In the conventional setting of $P4_2/m$, a point belonging to this Wyckoff position is given by x, y, 0 and one finds that the orbit of this point in special position is characteristic, *i.e.* its eigensymmetry group is just $P4_2/m$.

If we assume that the metric of the space group is not special, the eigensymmetry group is restricted to the same crystal family (for the definition of 'specialized' metrics, *cf.* Section 1.3.4.3 and Chapter 3.5). Therefore, a space group $\mathcal{G}$ for which the point group is a holohedry can only have non-characteristic orbits by additional translations, *i.e.* extraordinary orbits. However, if we allow specialized metrics, the eigensymmetry group may belong to a higher crystal family. For example, if a space group belongs to the orthorhombic family, but the unit cell has equal parameters

$a = b$, then the eigensymmetry group of an orbit can belong to the tetragonal family.

Note: A space group $\mathcal{G}$ is equal to the intersection of the eigensymmetry groups of the orbits of all its positions. If none of the positions of a space group $\mathcal{G}$ gives rise to a characteristic orbit, this means that each single orbit under $\mathcal{G}$ does not have $\mathcal{G}$ as its symmetry group, but a larger group that contains $\mathcal{G}$ as a proper subgroup. It may thus be necessary to have the union of at least two orbits under $\mathcal{G}$ to obtain a structure that has precisely $\mathcal{G}$ as its group of symmetry operations.

Examples

(1) For the group $\mathcal{G}$ of type *Pmmm* (47) all Wyckoff positions with no further special values of the coordinates give rise to characteristic orbits, because the point group of $\mathcal{G}$ is a holohedry and the general coordinates allow no further translations. However, there are various 'specializations' of the positions that give rise to extraordinary orbits. For example, setting x to the special value $\frac{1}{4}$ for the general position introduces the additional translation $t(\frac{1}{2}, 0, 0)$. In fact, for all positions in which the first coordinate has no specified value (positions $2i$–$2l$, $4w$–$4z$, 8α), setting $x = \frac{1}{4}$ introduces the translation $t(\frac{1}{2}, 0, 0)$ and thus gives rise to an extraordinary orbit. In all these cases, the resulting eigensymmetry group is of type *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$.

(2) For the group $\mathcal{G}$ of type *Pmm*2 (25) no Wyckoff position gives rise to a characteristic orbit, because this is a polar group (with respect to the c axis). Any orbit of a point with third coordinate z allows an additional mirror plane normal to the c axis and located at $0, 0, z$. For example, the general position gives rise to a non-characteristic orbit with eigensymmetry group *Pmmm* (47). Since the general coordinates allow no additional translation, this is not an extraordinary orbit. However, setting $x = \frac{1}{4}$ for the general position introduces the translation $t(\frac{1}{2}, 0, 0)$ (as in the above example) and thus gives rise to an extraordinary orbit. The eigensymmetry group is *Pmmm* with primitive lattice basis $\frac{1}{2}\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$.

On the other hand, the special positions x, 0, z (Wyckoff position $2e$) and $x, \frac{1}{2}, z$ (Wyckoff position $2f$) both have the same eigensymmetry group as the general position and setting $x = \frac{1}{4}$ for each, giving $\frac{1}{4}, 0, z$ and $\frac{1}{4}, \frac{1}{2}, z$, results in these positions having the same eigensymmetry group as the $\frac{1}{4}, y, z$ case of the general position.

(3) For a group $\mathcal{G}$ of type $P\bar{4}c2$ (116) the general-position coordinates are

(1) x, y, z	(2) $\bar{x}, \bar{y}, z$	(3) $y, \bar{x}, \bar{z}$	(4) $\bar{y}, x, \bar{z}$
(5) $x, \bar{y}, z + \frac{1}{2}$	(6) $\bar{x}, y, z + \frac{1}{2}$	(7) $y, x, \bar{z} + \frac{1}{2}$	(8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$

A point x, y, z in a general position does not give rise to an extraordinary orbit because, owing to the general coordinates, there can not be any additional translation. Furthermore, the point group $\bar{4}m2$ of $\mathcal{G}$ has index 2 in the holohedry $4/mmm$. Thus, in order to have a non-characteristic orbit one would require an inversion in some point as an additional operation. But an inversion in p_1, p_2, p_3 would map x, y, z to $\bar{x} + 2p_1, \bar{y} + 2p_2, \bar{z} + 2p_3$ and no such point is contained in the orbit for generic x, y, z. The point x, y, z therefore gives rise to a characteristic orbit.

However, if the point in a general position is chosen with $x = y$, one indeed obtains an additional inversion at $0, 0, \frac{1}{4}$ which maps x, x, z to the orbit point $\bar{x}, \bar{x}, \bar{z} + \frac{1}{2}$ (general position point No. 8). This orbit thus is non-characteristic, but it is not extraordinary, since no additional translation is introduced. The eigensymmetry group obtained is $P4_2/mcm$ (132).

On the other hand, if the general position is chosen with $y = 0$, no additional inversion is obtained, but the translation by $\frac{1}{2}\mathbf{c}$ maps $x, 0, z$ to $x, 0, z + \frac{1}{2}$ (general-position point No. 5). The position $x, 0, z$ therefore gives rise to an extraordinary orbit with eigensymmetry group $P\bar{4}m2$ (115).

Knowledge of the eigensymmetry groups of the different positions for a group is of utmost importance for the analysis of diffraction patterns. Atoms in positions that give rise to non-characteristic orbits, in particular extraordinary orbits, may cause systematic absences that are not explained by the space-group operations. These absences are specified as *special reflection conditions* in the space-group tables of this volume, but only as long as no specialization of the coordinates is involved. For the latter case, the possible existence of systematic absences has to be deduced from the tables of noncharacteristic orbits. Reflection conditions are discussed in detail in Chapter 1.6.

Example

For the group $\mathcal{G}$ of type *Pccm* (49) the special position $\frac{1}{2}, 0, z$ (Wyckoff position $4p$) gives rise to an extraordinary orbit, since it allows the additional translation $\frac{1}{2}\mathbf{c}$. The special reflection condition corresponding to this additional translation is the integral reflection condition hkl: $l = 2n$. However, if the z coordinate in position $4p$ is set to $z = \frac{1}{8}$, the eigensymmetry group also contains the translation $\frac{1}{4}\mathbf{c}$. In this case, the special reflection condition becomes hkl: $l = 4n$.

1.4.5. Sections and projections of space groups

BY B. SOUVIGNIER

In crystallography, two-dimensional sections and projections of crystal structures play an important role, *e.g.* in structure determination by Fourier and Patterson methods or in the treatment of twin boundaries and domain walls. Planar sections of three-dimensional scattering density functions are used for finding approximate locations of atoms in a crystal structure. They are indispensable for the location of Patterson peaks corresponding to vectors between equivalent atoms in different asymmetric units (the Harker vectors).

1.4.5.1. Introduction

A two-dimensional section of a crystal pattern takes out a slice of a crystal pattern. In the mathematical idealization, this slice is regarded as a two-dimensional plane, allowing one, however, to distinguish its upper and lower side. Depending on how the slice is oriented with respect to the crystal lattice, the slice will be invariant by translations of the crystal pattern along zero, one or two linearly independent directions. A section resulting in a slice with two-dimensional translational symmetry is called a *rational section* and is by far the most important case for crystallography.

Because the slice is regarded as a two-sided plane, the symmetries of the full crystal pattern that leave the slice invariant fall into two types:

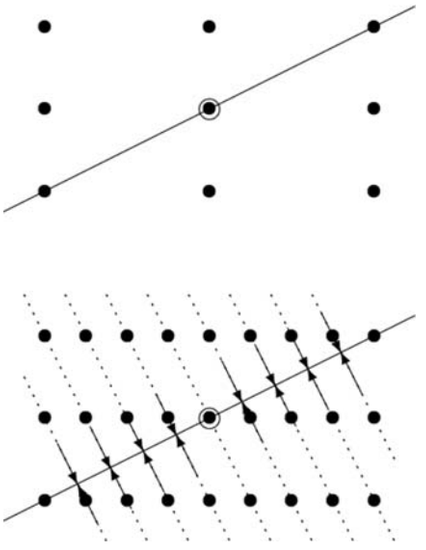

Figure 1.4.5.1
Duality between section and projection.

(i) If a symmetry operation of the slice maps its upper side to the upper side, a vector normal to the slice is fixed.
(ii) If a symmetry operation of the slice maps the upper side to the lower side, a vector normal to the slice is mapped to its opposite and the slice is turned upside down.

Therefore, the symmetries of two-dimensional rational sections are described by *layer groups*, *i.e.* subgroups of space groups with a two-dimensional translation lattice. Layer groups are *subperiodic groups* and for their elaborate discussion we refer to Chapter 1.7 and *IT* E (2010).

Analogous to two-dimensional sections of a crystal pattern, one can also consider the penetration of crystal patterns by a straight line, which is the idealization of a one-dimensional section taking out a rod of the crystal pattern. If the penetration line is along the direction of a translational symmetry of the crystal pattern, the rod has one-dimensional translational symmetry and its group of symmetries is a *rod group*, *i.e.* a subgroup of a space group with a one-dimensional translation lattice. Rod groups are also subperiodic groups, *cf. IT* E for their detailed treatment and listing.

A projection along a direction **d** into a plane maps a point of a crystal pattern to the intersection of the plane with the line along **d** through the point. If the projection direction is not along a rational lattice direction, the projection of the crystal pattern will contain points with arbitrarily small distances and additional restrictions are required to obtain a discrete pattern (*e.g.* the cut-and-project method used in the context of quasicrystals). We avoid any such complication by assuming that **d** is along a rational lattice direction. Furthermore, one is usually only interested in *orthogonal* projections in which the projection direction is perpendicular to the projection plane. This has the effect that spheres in three-dimensional space are mapped to circles in the projection plane.

Although it is also possible to regard the projection plane as a two-sided plane by taking into account from which side of the plane a point is projected into it, this is usually not done. Therefore, the symmetries of projections are described by ordinary plane groups.

Sections and projections are related by the *projection–slice theorem* (Bracewell, 2003) of Fourier theory: A section in reciprocal space containing the origin (the so-called zero layer) corresponds to a projection in direct space and *vice versa*. The projection direction in the one space is normal to the slice in the other space. This correspondence is illustrated schematically in Fig. 1.4.5.1. The top part shows a rectangular lattice with $b/a = 2$ and a slice along the line defined by $2x + y = 0$. Normalizing $a = 1$, the distance between two neighbouring lattice points in the slice is $\sqrt{5}$. If the pattern is restricted to this slice, the points of the corresponding diffraction pattern in reciprocal space must have distance $1/\sqrt{5}$ and this is precisely obtained by projecting the lattice points of the reciprocal lattice onto the slice.

The different, but related, viewpoints of sections and projections can be stated in a simple way as follows: For a section perpendicular to the c axis, only those points of a crystal pattern are considered which have z coordinate equal to a fixed value z_0 or in a small interval around z_0. For a projection along the c axis, all points of the crystal pattern are considered, but their z coordinate is simply ignored. This means that all points of the crystal pattern that differ only by their z coordinate are regarded as the same point.

1.4.5.2. Sections

For a space group $\mathcal{G}$ and a point X in the three-dimensional point space $\mathbb{E}^3$, the site-symmetry group of X is the subgroup of operations of $\mathcal{G}$ that fix X. Analogously, one can also look at the subgroup of operations fixing a one-dimensional line or a two-dimensional plane. If the line is along a rational direction, it will be fixed at least by the translations of $\mathcal{G}$ along that direction. However, it may also be fixed by a symmetry operation that reverses the direction of the line. The resulting subgroup of $\mathcal{G}$ that fixes the line is a *rod group*.

Similarly, a plane having a normal vector along a rational direction is fixed by translations of $\mathcal{G}$ corresponding to a two-dimensional lattice. Again, the plane may also be fixed by additional symmetry operations, *e.g.* by a twofold rotation around an axis lying in the plane, by a rotation around an axis normal to the plane or by a reflection in the plane.

Definition

A *rational planar section* of a crystal pattern is the intersection of the crystal pattern with a plane containing two linearly independent translation vectors of the crystal pattern. The intersecting plane is called the *section plane*.

A *rational linear section* of a crystal pattern is the intersection of the crystal pattern with a line containing a translation vector of the crystal pattern. The intersecting line is called the *penetration line*.

A planar section is determined by a vector **d** which is perpendicular to the section plane and a continuous parameter s, called the *height*, which gives the position of the plane on the line along **d**.

A linear section is specified by a vector **d** parallel to the penetration line and a point in a plane perpendicular to **d** giving the intersection of the line with that plane.

Definition

(i) The symmetry group of a planar section of a crystal pattern is the subgroup of the space group $\mathcal{G}$ of the crystal pattern that leaves the section plane invariant as a whole.

If the section is a rational section, this symmetry group is a *layer group*, *i.e.* a subgroup of a space group which contains translations only in a two-dimensional plane.

(ii) The symmetry group of a linear section of a crystal pattern is the subgroup of the space group $\mathcal{G}$ of the crystal pattern that leaves the penetration line invariant as a whole.

If the section is a rational section, this symmetry group is a *rod group*, *i.e.* a subgroup of a space group which contains translations only along a one-dimensional line.

From now on we will only consider rational sections and omit this attribute. Moreover, we will concentrate on the case of planar sections, since this is by far the most relevant case for crystallographic applications. The treatment of one-dimensional sections is analogous, but in general much easier.

Let **d** be a vector perpendicular to the section plane. In most cases, **d** is chosen as the shortest lattice vector perpendicular to the section plane. However, in the triclinic and monoclinic crystal family this may not be possible, since the translations of the crystal pattern may not contain a vector perpendicular to the section plane. In that case, we assume that **d** captures the periodicity of the crystal pattern perpendicular to the section plane. This is achieved by choosing **d** as the shortest non-zero projection of a lattice vector to the line through the origin which is perpendicular to the section plane. Because of the periodicity of the crystal pattern along **d**, it is enough to consider heights s with $0 \leq s < 1$, since for an integer m the sectional layer groups at heights s and $s + m$ are conjugate subgroups of $\mathcal{G}$. This is a consequence of the orbit–stabilizer theorem in Section 1.1.7, applied to the group $\mathcal{G}$ acting on the planes in $\mathbb{E}^3$. The layer at height s is mapped to the layer at height $s + m$ by the translation through m**d**. Thus, the two layers lie in the same orbit under $\mathcal{G}$. According to the orbit–stabilizer theorem, the corresponding stabilizers, being just the layer groups at heights s and $s + m$, are then conjugate by the translation through m**d**.

Since we assume a rational section, the sectional layer group will always contain translations along two independent directions $\mathbf{a}'$, $\mathbf{b}'$ which, we assume, form a crystallographic basis for the lattice of translations fixing the section plane. The points in the section plane at height s are then given by $x\mathbf{a}' + y\mathbf{b}' + s\mathbf{d}$. In order to determine whether the sectional layer group contains additional symmetry operations which are not translations, the following simple remark is crucial:

Let g be an operation of a sectional layer group. Then the rotational part of g maps **d** either to $+\mathbf{d}$ or to $-\mathbf{d}$. In the former case, g is side-preserving, in the latter case it is side-reversing. Moreover, since the section plane remains fixed under g, the vectors $\mathbf{a}'$ and $\mathbf{b}'$ are mapped to linear combinations of $\mathbf{a}'$ and $\mathbf{b}'$ by the rotational part of g. Therefore, with respect to the (usually non-conventional) basis $\mathbf{a}'$, $\mathbf{b}'$, **d** of three-dimensional space and some choice of origin, the operation g has an augmented matrix of the form

$$\left(\begin{array}{ccc|c} r_{11} & r_{12} & 0 & t_1 \\ r_{21} & r_{22} & 0 & t_2 \\ 0 & 0 & r_{33} & t_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Here, $r_{33} = \pm 1$. Moreover, if $r_{33} = 1$, *i.e.* g is side-preserving, then t_3 is necessarily zero, since otherwise the plane is shifted along **d**. On the other hand, if $r_{33} = -1$, *i.e.* g is side-reversing, then a plane situated at height s along **d** is only fixed if $t_3 = 2s$.

Table 1.4.5.1
Coset representatives of $Pmn2_1$ (31) relative to its translation subgroup

Seitz symbol	Coordinate triplet	Description
$\{1\|0\}$	x, y, z	Identity
$\{2_{001}\|\frac{1}{2}, 0, \frac{1}{2}\}$	$\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	Twofold screw rotation with axis along [001]
$\{m_{010}\|\frac{1}{2}, 0, \frac{1}{2}\}$	$x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$	n-glide reflection with normal vector along [010]
$\{m_{100}\|0\}$	$\bar{x}, y, z$	Reflection with normal vector along [100]

From these considerations it is straightforward to determine the conditions under which a space-group operation belongs to a certain sectional layer group (excluding translations):

The side-preserving operations will belong to the sectional layer groups for all planes perpendicular to **d**, independent of the height s:

(i) rotations with axis parallel to **d**;
(ii) reflections with normal vector perpendicular to **d**;
(iii) glide reflections with normal vector and glide vector perpendicular to **d**.

Side-reversing operations will only occur in the sectional layer groups for planes at special heights along **d**:

(i) inversion with inversion point in the section plane;
(ii) twofold rotations or twofold screw rotations with rotation axis in the section plane;
(iii) reflections or glide reflections through the section plane with glide vector perpendicular to **d**;
(iv) rotoinversions with axis parallel to **d** and inversion point in the section plane.

Note that, because of the periodicity along **d**, a side-reversing operation that occurs at height s gives rise to a side-reversing operation of the same type occurring at height $s + \frac{1}{2}$: if g is a side-reversing symmetry operation fixing a layer at height s, then g maps a point in the layer at height $s + \frac{1}{2}$ with coordinates $x, y, s + \frac{1}{2}$ (with respect to the layer-adapted basis $\mathbf{a}', \mathbf{b}', \mathbf{d}$) to a point with coordinates $x', y', s - \frac{1}{2}$ and hence the composition $t_{\mathbf{d}}g$ of g with the translation by **d** maps $x, y, s + \frac{1}{2}$ to $x', y', s + \frac{1}{2}$, *i.e.* it fixes the layer at height $s + \frac{1}{2}$. This shows that the composition with the translation by **d** provides a one-to-one correspondence between the side-reversing symmetry operations in the layer group at height s with those at height $s + \frac{1}{2}$.

If a section allows any side-reversing symmetry at all, then the side-preserving symmetries of the section form a subgroup of index 2 in the sectional layer group. Since the side-preserving symmetries exist independently of the height parameter s, the full sectional layer group is always generated by the side-preserving subgroup and either none or a single side-reversing symmetry.

Summarizing, one can conclude that for a given space group the interesting sections are those for which the perpendicular vector **d** is parallel or perpendicular to a symmetry direction of the group, *e.g.* an axis of a rotation or rotoinversion or the normal vector of a reflection or glide reflection.

Example

Consider the space group $\mathcal{G}$ of type $Pmn2_1$ (31). In its standard setting, the cosets of $\mathcal{G}$ relative to the translation subgroup are represented by the operations given in Table 1.4.5.1.

Since this is an orthorhombic group, it is natural to consider sections along the coordinate axes. The space-group diagrams displayed in Fig. 1.4.5.2, which show the orthogonal projections of the symmetry elements along these directions, are very helpful.

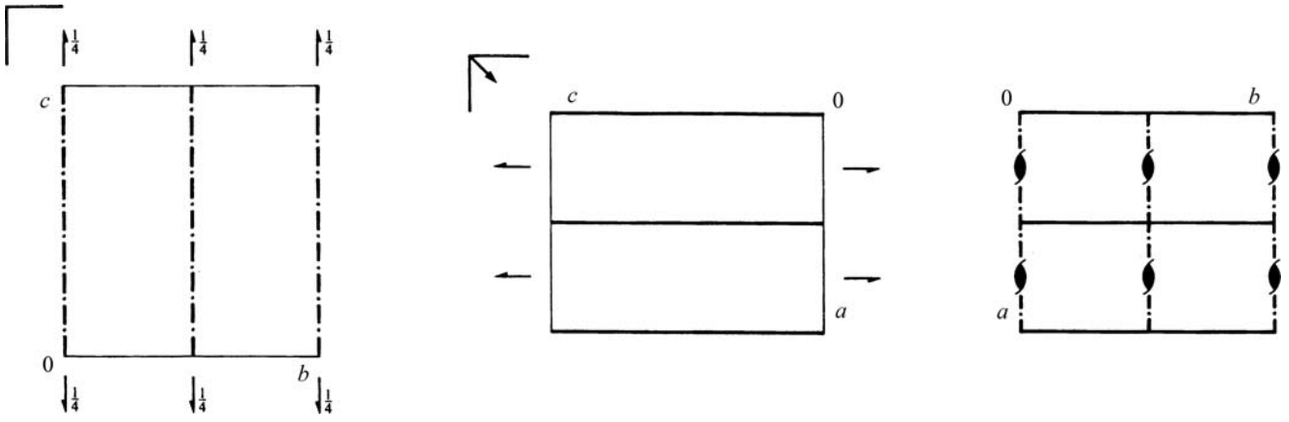

Figure 1.4.5.2
Symmetry-element diagrams for the space group $Pmn2_1$ (31) for orthogonal projections along [100] (left), [010] (middle) and [001] (right).

d *along* [100]: A point x, y, z in a plane perpendicular to the coordinate axis along [100] is mapped to a point x', y', z' in the same plane if $x' = x$, *i.e.* if $x' - x = 0$.

A general operation from the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ maps a point with coordinates x, y, z to a point with coordinates $x' = \bar{x} + \frac{1}{2} + u_1$, $y' = \bar{y} + u_2$, $z' = z + \frac{1}{2} + u_3$ for integers u_1, u_2, u_3. One has $x' - x = -2x + \frac{1}{2} + u_1$ which becomes zero for $x = \frac{1}{4}$ (and $u_1 = 0$) and $x = \frac{3}{4}$ (and $u_1 = 1$), thus operations from the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ fix planes at heights $s = \frac{1}{4}$ and $\frac{3}{4}$. In the left-hand diagram in Fig. 1.4.5.2, the symmetry elements to which these operations belong are indicated by the half-arrows, the label $\frac{1}{4}$ indicating that they are at level $x = \frac{1}{4}$ and $x = \frac{3}{4}$.

An operation from the coset of $\{m_{010}|\frac{1}{2}, 0, \frac{1}{2}\}$ maps x, y, z to $x' = x + \frac{1}{2} + u_1$, $y' = \bar{y} + u_2$, $z' = z + \frac{1}{2} + u_3$ and one has $x' - x = \frac{1}{2} + u_1$. Since this is never zero, no operation from this coset fixes a plane perpendicular to [100].

Finally, an operation from the coset of $\{m_{100}|0\}$ maps x, y, z to $x' = \bar{x} + u_1$, $y' = y + u_2$, $z' = z + u_3$ and one has $x' - x = -2x + u_1$, which becomes zero for $x = 0$ (and $u_1 = 0$) and $x = \frac{1}{2}$ (and $u_1 = 1$). Thus, operations from the coset of $\{m_{100}|0\}$ fix planes at heights $s = 0$ and $\frac{1}{2}$. The symmetry elements of these reflections with mirror plane parallel to the projection plane are indicated by the right-angle symbol in the upper left corner of the left-hand diagram in Fig. 1.4.5.2.

The sectional layer groups are thus layer groups of type $pm11$ (layer group No. 4 with symbol $p11m$ in a non-standard setting) for $s = 0$ and $s = \frac{1}{2}$, of type $p112_1$ (layer group No. 9 with symbol $p2_111$ in a non-standard setting) for $s = \frac{1}{4}$ and $s = \frac{3}{4}$ and of type $p1$ (layer group No. 1) for all other s between 0 and 1. The side-preserving operations are in all cases just the translations.

It is worthwhile noting that in many cases most of the information about the sectional layer groups can be read off the space-group diagrams. In the present example, the left-hand diagram in Fig. 1.4.5.2 displays the twofold screw rotation at height $s = \frac{1}{4}$ (and thus also at $s = \frac{3}{4}$) and the reflection at height $s = 0$ (and thus also at $s = \frac{1}{2}$). On the other hand, the n glide, indicated by the dashed-dotted lines in the diagram, does not give rise to an element of the sectional layer group, because its glide vector has a component along the [100] direction and can thus not fix any layer along this direction.

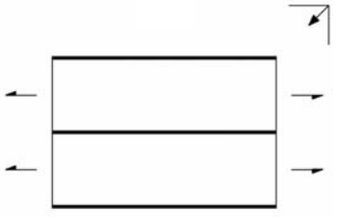

Figure 1.4.5.3
Symmetry-element diagram for the layer group $pm2_1n$ (32).

d *along* [010]: A point x, y, z in a plane perpendicular to the coordinate axis along [010] is mapped to a point x', y', z' in the same plane if $y' = y$, *i.e.* if $y' - y = 0$.

From the calculations above one sees that for operations in the coset of $\{m_{100}|0\}$ one has $y' - y = u_2$, hence operations in this coset fix the plane for any value of s and are side-preserving operations. In the middle diagram in Fig. 1.4.5.2 the symmetry elements for these reflections are indicated by the horizontal solid lines.

For the operations in the coset of $\{2_{001}|\frac{1}{2}, 0, \frac{1}{2}\}$ one has $y' - y = -2y + u_2$, and so these operations fix planes only for $s = 0$ and $s = \frac{1}{2}$. The same is true for the operations in the coset of $\{m_{010}|\frac{1}{2}, 0, \frac{1}{2}\}$, because here one also has $y' - y = -2y + u_2$. The symmetry elements to which the screw rotations belong are indicated by the half arrows in the middle diagram of Fig. 1.4.5.2, and the symmetry elements for the glide reflections are symbolized by the right angle with diagonal arrow in the upper left corner, indicating that the geometric element is a diagonal glide plane.

The sectional layer groups are thus of type $pmn2_1$ (layer group No. 32 with symbol $pm2_1n$ in a non-standard setting) for $s = 0, \frac{1}{2}$ and of type $pm11$ (layer group No. 11) for all other s. The group of side-preserving operations is in all cases of type $pm11$.

In Fig. 1.4.5.3 the diagram of the symmetry elements for the layer group $pm2_1n$ (layer group No. 32) is displayed. It coincides with the middle diagram in Fig. 1.4.5.2 (up to the placement of the symbol for the diagonal glide plane), showing that in this case the sectional layer groups can also be read off directly from the space-group diagrams.

d *along* [001]: A point x, y, z in a plane perpendicular to the coordinate axis along [001] is mapped to a point x', y', z' in the same plane if $z' = z$, *i.e.* if $z' - z = 0$.

As in the case of **d** along [010], operations in the coset of $\{m_{100}|0\}$ fix such a plane for any value of s, since $z' - z = u_3$.

Again, these are side-preserving operations. The symmetry elements to which these reflections belong are indicated by the horizontal solid lines in the right-hand diagram in Fig. 1.4.5.2. For the operations in the cosets of $\{2_{001}|\frac{1}{2},0,\frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2},0,\frac{1}{2}\}$ one has $z'-z=\frac{1}{2}+u_3$, which is never zero (for an integer u_3), and so operations in these cosets never fix a plane perpendicular to [001].

Thus, for any value of s the sectional layer group is of type $pm11$ (layer group No. 11) and contains only side-preserving operations.

1.4.5.3. Projections

As we have seen, a section of a crystal pattern is determined by a vector **d** and a height s along this vector. Choosing two vectors $\mathbf{a}'$ and $\mathbf{b}'$ perpendicular to **d**, the points of the section plane at height s are precisely given by the vectors $x\mathbf{a}'+y\mathbf{b}'+s\mathbf{d}$. In contrast to that, a *projection* of a crystal pattern along **d** is obtained by mapping an arbitrary point $x\mathbf{a}'+y\mathbf{b}'+z\mathbf{d}$ to the point $x\mathbf{a}'+y\mathbf{b}'$ of the plane spanned by $\mathbf{a}'$ and $\mathbf{b}'$, thereby ignoring the coordinate along the **d** direction.

Definition

In a *projection* of a crystal pattern along the *projection direction* **d**, a point X of the crystal pattern is mapped to the intersection of the line through X along **d** with a fixed plane perpendicular to **d**.

One may think of the projection plane as the plane perpendicular to **d** and containing the origin, but every plane perpendicular to **d** will give the same result.

Let L be the line along **d**. If a symmetry operation g of a space group $\mathcal{G}$ maps L to a line parallel to L, then g maps every plane perpendicular to **d** again to a plane perpendicular to **d**. This means that points that are projected to a single point (*i.e.* points on a line parallel to L) are mapped by g to points that are again projected to a single point and thus the operation g gives rise to a symmetry of the projection of the crystal pattern. Conversely, an operation g that maps L to a line that is inclined to L does not result in a symmetry of the projection, since the points on L are projected to a single point, whereas the image points under g are projected to a line. In summary, the operations of $\mathcal{G}$ that map L to a line parallel to L give rise to symmetries of the projection forming a *plane group*, sometimes called a wallpaper group.

Let $\mathcal{H}$ be the subgroup of $\mathcal{G}$ consisting of those $g\in\mathcal{G}$ mapping the line L to a line parallel to L, then $\mathcal{H}$ is called the *scanning group along* **d**. The scanning group $\mathcal{H}$ can be read off a coset decomposition $\mathcal{G}=g_1\mathcal{T}\cup\cdots\cup g_s\mathcal{T}$ relative to the translation subgroup $\mathcal{T}$ of $\mathcal{G}$. Since translations map lines to parallel lines, one only has to check whether a coset representative g_i maps L to a line parallel to L. This is precisely the case if the linear part of g_i maps **d** to **d** or to $-\mathbf{d}$. Therefore, $\mathcal{H}$ is the union of those cosets $g_i\mathcal{T}$ relative to $\mathcal{T}$ for which the linear part of g_i maps **d** to **d** or to $-\mathbf{d}$.

If the operations of a space group $\mathcal{G}$ are written as augmented matrices with respect to a (usually non-conventional) basis $\mathbf{a}'$, $\mathbf{b}'$, **d** such that $\mathbf{a}'$ and $\mathbf{b}'$ are perpendicular to **d**, then an operation g of the scanning group $\mathcal{H}$ is of the form

$$g=\left(\begin{array}{ccc|c} r_{11} & r_{12} & 0 & t_1\\ r_{21} & r_{22} & 0 & t_2\\ 0 & 0 & r_{33} & t_3\\ \hline 0 & 0 & 0 & 1\end{array}\right)$$

with $r_{33}=\pm1$ (just as for planar sections). Then the action of g on the projection along **d** is obtained by ignoring the z coordinate, *i.e.* by cutting out the upper 2×2 block of the linear part and the first two components of the translation part. This gives rise to the plane-group operation

$$g'=\left(\begin{array}{cc|c} r_{11} & r_{12} & t_1\\ r_{21} & r_{22} & t_2\\ \hline 0 & 0 & 1\end{array}\right).$$

The mapping that assigns to each operation g of the scanning group its action g' on the projection is in fact a homomorphism from $\mathcal{H}$ to a plane group and the kernel $\mathcal{K}$ of this homomorphism are the operations of the form

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & r_{33} & t_3\\ \hline 0 & 0 & 0 & 1\end{array}\right),$$

i.e. translations along **d** and reflections with normal vector parallel to **d**.

Definition

The symmetry group of the projection along the projection direction **d** is the plane group of actions on the projection of those operations of $\mathcal{G}$ that map the line L along **d** to a line parallel to L.

This group is isomorphic to the quotient group of the scanning group $\mathcal{H}$ along **d** by the group $\mathcal{K}$ of translations along **d** and reflections with normal vector parallel to **d**.

Example

We consider again the space group $\mathcal{G}$ of type $Pmn2_1$ (31) for which the augmented matrices of the coset representatives with respect to the translation subgroup (in the standard setting) are given by

$$\{1|0\}=\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ \hline 0 & 0 & 0 & 1\end{array}\right),$$

$$\{2_{001}|\tfrac{1}{2},0,\tfrac{1}{2}\}=\left(\begin{array}{ccc|c} -1 & 0 & 0 & \frac{1}{2}\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & \frac{1}{2}\\ \hline 0 & 0 & 0 & 1\end{array}\right)$$

$$\{m_{010}|\tfrac{1}{2},0,\tfrac{1}{2}\}=\left(\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2}\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & \frac{1}{2}\\ \hline 0 & 0 & 0 & 1\end{array}\right),$$

$$\{m_{100}|0\}=\left(\begin{array}{ccc|c} -1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ \hline 0 & 0 & 0 & 1\end{array}\right).$$

Since the linear parts of all four matrices are diagonal matrices, the scanning group for projections along the coordinate axes is always the full group $\mathcal{G}$.

For the projection along the direction [100], one has to cut out the lower 2×2 part of the linear parts and the second and third component of the translation part, thus choosing $\mathbf{a}' = \mathbf{b}, \mathbf{b}' = \mathbf{c}$ as a basis for the projection plane. This gives as matrices for the projected operations

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

in which the third and fourth operations are clearly redundant and which is thus a plane group of type $p1g1$ (plane group No. 4 with short symbol pg).

The projection along the direction [010] gives for the basis $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{c}$ of the projection plane (thus picking out the first and third rows and columns) the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where the second matrix is the product of the third and fourth. The third operation is a centring translation, the fourth a reflection, thus the resulting plane group is of type $c1m1$ (plane group No. 5 with short symbol cm).

Finally, the projection along the direction [001] results for the basis $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{b}$ of the projection plane in the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \quad \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where again the second matrix is the product of two others. The third operation is a glide reflection and the fourth is a reflection, thus the corresponding plane group is of type $p2mg$ (plane group No. 7). Note that in order to obtain the plane group $p2mg$ in its standard setting, the origin has to be shifted to $\frac{1}{4}, 0$ (with respect to the plane basis $\mathbf{a}', \mathbf{b}'$).

As for the sectional layer groups, the typical projection directions considered are symmetry directions of the space group $\mathcal{G}$, *i.e.* directions along rotation or screw axes or normal to reflection or glide planes. In order to relate the coordinate system of the plane group to that of the space group, not only the basis vectors $\mathbf{a}', \mathbf{b}'$ perpendicular to the projection direction $\mathbf{d}$ have to be given, but also the origin for the plane group. This is done by specifying a line parallel to the projection direction which is projected to the origin of the plane group in its conventional setting. The space-group tables list the plane groups for the projections along symmetry directions of the group in the block 'Symmetry of special projections'.

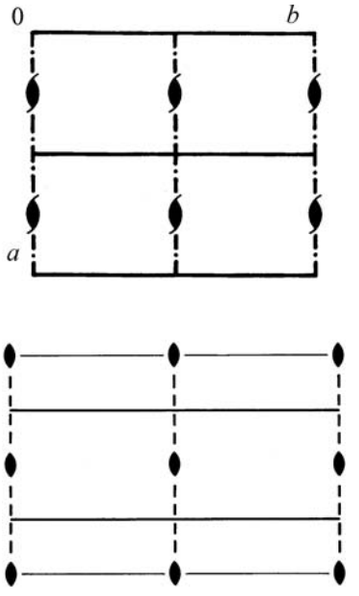

Figure 1.4.5.4
Orthogonal projection along [001] of the symmetry-element diagram for $Pmn2_1$ (31) (top) and the diagram for plane group $p2mg$ (7) (bottom).

It is not hard to determine the corresponding types of plane-group operations for the different types of space-group operations, as is shown by the following list of simple rules:

(i) a translation becomes a translation (possibly the identity);
(ii) an inversion becomes a twofold rotation;
(iii) a k-fold rotation or screw rotation with axis parallel to $\mathbf{d}$ becomes a k-fold rotation;
(iv) a three-, four- or sixfold rotoinversion with axis parallel to $\mathbf{d}$ becomes a six-, four- or threefold rotation, respectively;
(v) a reflection or glide reflection with normal vector parallel to $\mathbf{d}$ becomes a translation (possibly the identity);
(vi) a twofold rotation and a screw rotation with axis perpendicular to $\mathbf{d}$ become a reflection and glide reflection, respectively;
(vii) a reflection or a glide reflection with normal vector perpendicular to $\mathbf{d}$ becomes a reflection or glide reflection depending on whether there is a glide component perpendicular to $\mathbf{d}$ or not.

The relationship between the symmetry operations in three-dimensional space and the corresponding symmetry operations of a projection as listed above can be seen directly in the diagrams of the corresponding groups. In Fig. 1.4.5.4, the top diagram shows the orthogonal projection of the symmetry-element diagram of $Pmn2_1$ along the [001] direction and the bottom diagram shows the diagram for the plane group $p2mg$, which is precisely the symmetry group of the projection of $Pmn2_1$ along [001]. Firstly, one sees immediately that in order to match the two diagrams, the origin in the projection plane has to be shifted to $\frac{1}{4}, 0$ (as already noted in the example above). Secondly, keeping in mind that the projection direction $\mathbf{d}$ is perpendicular to the drawing plane, one sees the correspondence between the twofold screw rotations in $Pmn2_1$ with the twofold rotations in $p2mg$ [rule (iii)], the correspondence between the

reflections with normal vector perpendicular to **d** in $Pmn2_1$ and the reflections in $p2mg$ [rule (vii)] and the correspondence between the diagonal glide reflections in $Pmn2_1$ (indicated by the dot-dash lines) and the glide reflections in $p2mg$ {rule (vii); note that the diagonal glide vector has a component perpendicular to the projection direction [001]}.

Example

Let $\mathcal{G}$ be a space group of type $P\bar{4}b2$ (117), then the interesting projection directions (*i.e.* symmetry directions) are [100], [010], [001], [110] and [$\bar{1}$10]. However, the directions [100] and [010] are symmetry-related by the fourfold rotoinversion and thus result in the same projection. The same holds for the directions [110] and [$\bar{1}$10]. The three remaining directions are genuinely different and the projections along these directions will be discussed in detail below. The corresponding information given in the space-group tables under the heading 'Symmetry of special projections' is reproduced in Fig. 1.4.5.5 for $P\bar{4}b2$.

Coset representatives of $\mathcal{G}$ relative to its translation subgroup can be extracted from the general-positions block in the space-group tables of $P\bar{4}b2$ and are given in Table 1.4.5.2.

d *along* [001]: The linear parts of all coset representatives map [001] to ±[001], and therefore the scanning group $\mathcal{H}$ is the full group $\mathcal{G}$. A conventional basis for the translations of the projection is $\mathbf{a}' = \mathbf{a}$ and $\mathbf{b}' = \mathbf{b}$. The operation g_3 acts as a fourfold rotation, g_5 acts as a glide reflection with normal vector $\mathbf{b}'$ and g_8 as a reflection with normal vector $\mathbf{a}' + \mathbf{b}'$. Thus, the resulting plane group has type $p4gm$ (plane group No. 12). The line parallel to the projection direction [001] which is projected to the origin of $p4gm$ in its conventional setting is the line 0, 0, z.

Again, it is instructive to look at the symmetry-element diagrams for the respective space and plane groups, as displayed in Fig. 1.4.5.6. The twofold rotations and fourfold rotoinversions with axis along [001] are turned into twofold rotations and fourfold rotations, respectively [rules (iii) and (iv)]. The glide reflections with both normal vector and glide vector perpendicular to [001] (dashed lines) result in glide reflections [rule (vii)]. The twofold rotations (full arrows) and screw rotations (half arrows) with rotation axis perpendicular to [001] give reflections and glide reflections, respectively [rule (vi)]. Note that the two diagrams can be matched directly, because the line 0, 0, z which is projected to the origin of $p4gm$ runs through the origin of $P\bar{4}b2$.

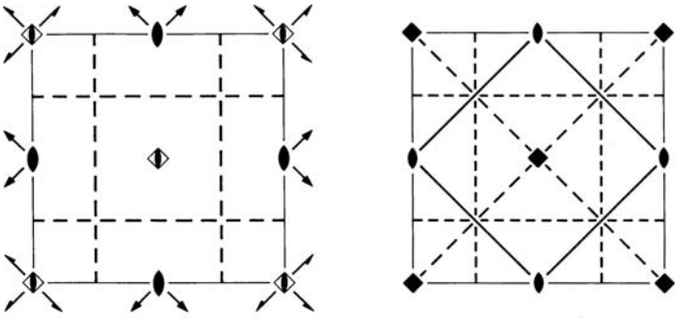

Figure 1.4.5.6
Orthogonal projection along [001] of the symmetry-element diagram for $P\bar{4}b2$ (117) (left) and the diagram for plane group $p4gm$ (12) (right).

Symmetry of special projections

Along [001] $p4gm$	Along [100] $p1m1$	Along [110] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\quad \mathbf{b}' = \mathbf{b}$	$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\quad \mathbf{b}' = \mathbf{c}$	$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}' = \mathbf{c}$
Origin at $0,0,z$	Origin at $x,0,0$	Origin at $x,x,0$

Figure 1.4.5.5
'Symmetry of special projections' block of $P\bar{4}b2$ (117) as given in the space-group tables.

d *along* [100]: Only the linear parts of the coset representatives g_1, g_2, g_5 and g_6 map [100] to ±[100], thus these four cosets form the scanning group $\mathcal{H}$ (which is of index 2 in $\mathcal{G}$). The operation g_6 acts as a translation by $\frac{1}{2}\mathbf{b}$, thus a conventional basis for the translations of the projection is $\mathbf{a}' = \frac{1}{2}\mathbf{b}$ and $\mathbf{b}' = \mathbf{c}$. The operation g_2 acts as a reflection with normal vector $\mathbf{a}'$ and g_5 acts as the same reflection composed with the translation $\mathbf{a}'$. The resulting plane group is thus of type $p1m1$ (plane group No. 3 with short symbol pm). The line which is mapped to the origin of $p1m1$ in its conventional setting is x, 0, 0.

d *along* [110]: Only the linear parts of the coset representatives g_1, g_2, g_7 and g_8 map [110] to ±[110], thus these four cosets form the scanning group $\mathcal{H}$ (of index 2 in $\mathcal{G}$). The translation by **b** is projected to a translation by $\frac{1}{2}(-\mathbf{a}+\mathbf{b})$, thus a conventional basis for the translations of the projection is $\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ and $\mathbf{b}' = \mathbf{c}$. The operation g_2 acts as a reflection with normal vector $\mathbf{a}'$, g_7 acts as a twofold rotation and g_8 acts as a reflection with normal vector $\mathbf{b}'$. The resulting plane group is thus of type $p2mm$ (plane group No. 6). The line parallel to the projection direction [110] that is mapped to the origin of $p2mm$ (in its conventional setting) is x, x, 0.

Note that for directions different from those considered above, additional non-trivial plane groups may be obtained. For example, for the projection direction $\mathbf{d} = [1\bar{1}1]$, the scanning group consists of the cosets of g_1 and g_7. The operation g_7 acts as a glide reflection and the resulting plane group is of type $c1m1$ (plane group No. 5).

Table 1.4.5.2
Coset representatives of $P\bar{4}b2$ (117) relative to its translation subgroup

	Coordinate triplet	Description
g_1:	x, y, z	Identity
g_2:	$\bar{x}, \bar{y}, z$	Twofold rotation with axis along [001]
g_3:	$y, \bar{x}, \bar{z}$	Fourfold rotoinversion with axis along [001]
g_4:	$\bar{y}, x, \bar{z}$	Fourfold rotoinversion with axis along [001]
g_5:	$x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$	Glide reflection with normal vector [010] and glide component along [100]
g_6:	$\bar{x}+\frac{1}{2}, y+\frac{1}{2}, z$	Glide reflection with normal vector [100] and glide component along [010]
g_7:	$y+\frac{1}{2}, x+\frac{1}{2}, \bar{z}$	Twofold screw rotation with axis parallel to [110]
g_8:	$\bar{y}+\frac{1}{2}, \bar{x}+\frac{1}{2}, \bar{z}$	Twofold rotation with axis parallel to [1$\bar{1}$0]

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1.5. Transformations of coordinate systems

H. Wondratschek, M. I. Aroyo, B. Souvignier and G. Chapuis

It is in general advantageous to refer crystallographic objects and their symmetries to the most appropriate coordinate system. The best coordinate system may be different for different steps of the calculations and for different objects which have to be considered simultaneously. Therefore, a change of the origin and/or the basis are frequently necessary when treating crystallographic problems, for example in the study of phase-transition phenomena, or in the comparison of crystal structures described with respect to different coordinate systems.

1.5.1. Origin shift and change of the basis[1]

By H. Wondratschek and M. I. Aroyo

1.5.1.1. Origin shift

Let a coordinate system be given with a basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and an origin O. Referred to this coordinate system, the column of coordinates of a point X is $\boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$ and the corresponding vector is $\mathbf{x} = x_1\mathbf{a} + x_2\mathbf{b} + x_3\mathbf{c}$. Referred to a new coordinate system, specified by the basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and the origin O', the column of coordinates of the point X is $\boldsymbol{x}' = \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix}$. Let $\boldsymbol{p} = \overrightarrow{OO'} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$ be the column of coefficients for the vector $\mathbf{p}$ from the old origin O to the new origin O', see Fig. 1.5.1.1.

For the columns $\boldsymbol{p} + \boldsymbol{x}' = \boldsymbol{x}$ holds, *i.e.*

$$\boldsymbol{x}' = \boldsymbol{x} - \boldsymbol{p} \quad \text{or} \quad \begin{pmatrix} x'_1 \\ x'_2 \\ x'_3 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} x_1 - p_1 \\ x_2 - p_2 \\ x_3 - p_3 \end{pmatrix}. \tag{1.5.1.1}$$

This can be written in the formalism of matrix–column pairs (*cf.* Section 1.2.2.3 for details of the matrix–column formalism) as

$$\boldsymbol{x}' = (\boldsymbol{I}, -\boldsymbol{p})\boldsymbol{x} \quad \text{or} \quad \boldsymbol{x}' = (\boldsymbol{I}, \boldsymbol{p})^{-1}\boldsymbol{x}, \tag{1.5.1.2}$$

where $(\boldsymbol{I}, \boldsymbol{p})$ represents the translation corresponding to the vector $\mathbf{p}$ of the origin shift.

The vector $\mathbf{r}$ determined by the points X and Y (also known as a 'distance vector'), $\mathbf{x} + \mathbf{r} = \mathbf{y}$ (*cf.* Fig. 1.5.1.1), and thus with coefficients

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix},$$

shows a different transformation behaviour under the origin shift. From the diagram one reads the equations $\mathbf{p} + \mathbf{x}' = \mathbf{x}$, $\mathbf{x} + \mathbf{r} = \mathbf{y}$, $\mathbf{x}' + \mathbf{r} = \mathbf{y}'$, and thus

$$\mathbf{r} = \mathbf{y}' - \mathbf{x}' = \mathbf{y} - \mathbf{x}, \tag{1.5.1.3}$$

i.e. the vector coefficients of $\mathbf{r}$ are not affected by the origin shift.

Example

The description of a crystal structure is closely related to its space-group symmetry: different descriptions of the underlying space group, in general, result in different descriptions of the crystal structure. This example illustrates the comparison of two structure descriptions corresponding to different origin choices of the space group.

To compare the two structures it is not only necessary to apply the origin-shift transformation but also to adjust the selection of the representative atoms of the two descriptions.

In the Inorganic Crystal Structure Database (2012) (abbreviated as ICSD) one finds the following two descriptions of the mineral zircon $ZrSiO_4$:

(*a*) Wyckoff & Hendricks (1927), ICSD No. 31101, space group $I4_1/amd = D_{4h}^{19}$, No. 141, cell parameters a = 6.61 Å, c = 5.98 Å.

The coordinates of the atoms in the unit cell are (normalized so that $0 \le x_i < 1$):

Zr:	4*a*	0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{4}$ [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+]
Si:	4*b*	0, 0, $\frac{1}{2}$; 0, $\frac{1}{2}$, $\frac{3}{4}$ [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+]
O:	16*h*	0, 0.2, 0.34; 0.5, 0.3, 0.84; 0.8, 0.5, 0.59; 0.7, 0, 0.09; 0.5, 0.2, 0.41; 0, 0.3, 0.91; 0.7, 0.5, 0.16; 0.8, 0, 0.66 [and the same with ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$)+].

The coordinates of Zr and Si atoms indicate that the space-group setting corresponds to the origin choice 1 description of $I4_1/amd$ given in this volume, *i.e.* origin at $\bar{4}m2$ (*cf.* the space-group tables for $I4_1/amd$ in Chapter 2.3).

(*b*) Krstanovic (1958), ICSD No. 45520, space group $I4_1/amd = D_{4h}^{19}$, No. 141, cell parameters a = 6.6164 (5) Å, c = 6.0150 (5) Å.

The coordinates of the atoms in the unit cell are (normalized so that $0 \le x_i < 1$):

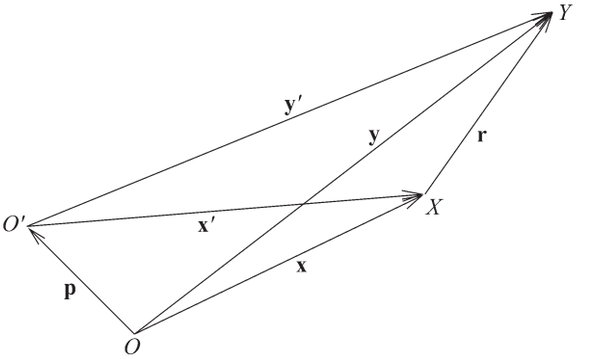

Figure 1.5.1.1
The coordinates of the points X (or Y) with respect to the old origin O are $\boldsymbol{x}$ ($\boldsymbol{y}$), and with respect to the new origin O' they are $\boldsymbol{x}'$ ($\boldsymbol{y}'$). From the diagram one reads $\mathbf{p} + \mathbf{x}' = \mathbf{x}$ and $\mathbf{p} + \mathbf{y}' = \mathbf{y}$.

[1] With Table 1.5.1.1 and Figs. 1.5.1.2 and 1.5.1.5–1.5.1.10 by H. Arnold.

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Zr:	4*a*	$0, \frac{3}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$ [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$]
Si:	4*b*	$0, \frac{1}{4}, \frac{3}{8}$; $0, \frac{3}{4}, \frac{5}{8}$ [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$]
O:	16*h*	0, 0.067, 0.198; 0.5, 0.933, 0.698; 0.183, 0.75, 0.448; 0.317, 0.25, 0.948; 0.5, 0.067, 0.302; 0, 0.933, 0.802; 0.317, 0.75, 0.052; 0.183, 0.25, 0.552 [and the same with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$].

The structure is described with respect to the origin choice 2 setting of $I4_1/amd$ specified in this volume as 'Origin at centre $(2/m)$ at $0, \frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$' (*cf.* the space-group tables for $I4_1/amd$ in Chapter 2.3).

In order to compare the different structure descriptions, the atomic coordinates of the origin choice 1 description are to be transformed to 'Origin at centre $2/m$', *i.e.* origin choice 2.

Origin choice 2 has coordinates $0, \frac{1}{4}, \frac{1}{8}$ referred to origin choice 1. Therefore, the change of coordinates consists of *subtracting* $\boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{4} \\ \frac{1}{8} \end{pmatrix}$ from the origin choice 1 values, *i.e.* leave the x coordinate unchanged, add $\frac{1}{4} = 0.25$ to the y coordinate and subtract $\frac{1}{8} = 0.125$ from the z coordinate [*cf.* equation (1.5.1.1)].

The transformed and normalized coordinates (so that $0 \leq x_i < 1$) are

(i) Zr: 4*a* $0, \frac{1}{4}, \frac{7}{8}$; $0, \frac{3}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{1}{4}, \frac{5}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{3}{8}$;

(ii) Si: 4*b* $0, \frac{1}{4}, \frac{3}{8}$; $0, \frac{3}{4}, \frac{5}{8}$; $\frac{1}{2}, \frac{1}{4}, \frac{1}{8}$; $\frac{1}{2}, \frac{3}{4}, \frac{7}{8}$;

(iii) O: 16*h* $0, 0.20 + 0.25, 0.34 - 0.125 = 0, 0.45, 0.215$.

This oxygen atom obviously does not correspond to the representative 0, 0.067, 0.198 given by Krstanovic (1958), but by adding the centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ it is seen to correspond to the second position with coordinates 0.5, 0.933, 0.698. The transformed (and normalized) coordinates of the rest of the oxygen atoms in the unit cell are:

0.5, 0.55, 0.715; 0.8, 0.75, 0.465; 0.7, 0.25, 0.965;
0.5, 0.45, 0.285; 0, 0.55, 0.785; 0.7, 0.75, 0.035;
0.8, 0.25, 0.535;

all also with $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})+$. The difference in the coordinates of the two descriptions could be explained by the difference in the accuracy of the two refinements.

1.5.1.2. Change of the basis

A change of the basis is described by a (3×3) matrix:

$$\boldsymbol{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}.$$

The matrix $\boldsymbol{P}$ relates the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ to the old basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ according to

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$
$$= (\mathbf{a}P_{11} + \mathbf{b}P_{21} + \mathbf{c}P_{31},\ \mathbf{a}P_{12} + \mathbf{b}P_{22} + \mathbf{c}P_{32},\ \mathbf{a}P_{13} + \mathbf{b}P_{23} + \mathbf{c}P_{33}). \quad (1.5.1.4)$$

The matrix $\boldsymbol{P}$ is often referred to as the *linear part* of the coordinate transformation and it describes a change of direction and/or length of the basis vectors. It is preferable to choose the matrix $\boldsymbol{P}$ in such a way that its determinant is positive: a negative determinant of $\boldsymbol{P}$ implies a change from a right-handed coordinate system to a left-handed coordinate system or *vice versa*. If $\det(\boldsymbol{P}) = 0$, then the new vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ are linearly dependent, *i.e.* they do not form a complete set of basis vectors.

For a point X (*cf.* Fig. 1.5.1.1), the vector $\overrightarrow{OX} = \mathbf{x}$ is

$$\mathbf{x} = \mathbf{a}x_1 + \mathbf{b}x_2 + \mathbf{c}x_3 = \mathbf{a}'x_1' + \mathbf{b}'x_2' + \mathbf{c}'x_3' \text{ or}$$
$$\mathbf{x} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = (\mathbf{a}', \mathbf{b}', \mathbf{c}') \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}.$$

By inserting equation (1.5.1.4) one obtains

$$\mathbf{x} = (\mathbf{a}', \mathbf{b}', \mathbf{c}') \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix}$$

or

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix},$$

i.e. $\boldsymbol{x} = \boldsymbol{P}\boldsymbol{x}'$ or $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} = (\boldsymbol{P}, \boldsymbol{o})^{-1}\boldsymbol{x}$, which is often written as

$$\boldsymbol{x}' = \boldsymbol{Q}\boldsymbol{x} = (\boldsymbol{Q}, \boldsymbol{o})\boldsymbol{x}. \quad (1.5.1.5)$$

Here the inverse matrix $\boldsymbol{P}^{-1}$ is designated by $\boldsymbol{Q}$, while $\boldsymbol{o}$ is the (3×1) column vector with zero coefficients. [Note that in equation (1.5.1.4) the sum is over the row (first) index of $\boldsymbol{P}$, while in equation (1.5.1.5), the sum is over the column (second) index of $\boldsymbol{Q}$.]

A selected set of transformation matrices $\boldsymbol{P}$ and their inverses $\boldsymbol{P}^{-1} = \boldsymbol{Q}$ that are frequently used in crystallographic calculations are listed in Table 1.5.1.1 and illustrated in Figs. 1.5.1.2 to 1.5.1.10.

Example

Consider an *F*-centred cell with conventional basis $\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F$ and a corresponding primitive cell with basis $\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P$, *cf.* Fig. 1.5.1.4. The transformation matrix $\boldsymbol{P}$ from the conventional basis to a primitive basis can either be deduced from Fig. 1.5.1.4 or can be read directly from Table 1.5.1.1: $\mathbf{a}_P = \frac{1}{2}(\mathbf{b}_F + \mathbf{c}_F)$, $\mathbf{b}_P = \frac{1}{2}(\mathbf{a}_F + \mathbf{c}_F)$, $\mathbf{c}_P = \frac{1}{2}(\mathbf{a}_F + \mathbf{b}_F)$, which in matrix notation is

$$(\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P) = (\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F)\boldsymbol{P} = (\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F) \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}.$$

The inverse matrix $\boldsymbol{P}^{-1} = \boldsymbol{Q}$ is also listed in Table 1.5.1.1 or can be deduced from Fig. 1.5.1.4. It is the matrix that describes the conventional basis vectors $\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F$ by linear combinations of $\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P$: $\mathbf{a}_F = -\mathbf{a}_P + \mathbf{b}_P + \mathbf{c}_P$, $\mathbf{b}_F = \mathbf{a}_P - \mathbf{b}_P + \mathbf{c}_P$, $\mathbf{c}_F = \mathbf{a}_P + \mathbf{b}_P - \mathbf{c}_P$, or

$$(\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F) = (\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P)\boldsymbol{P}^{-1} = (\mathbf{a}_P, \mathbf{b}_P, \mathbf{c}_P) \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}.$$

Correspondingly, the point coordinates transform as

Table 1.5.1.1
Selected 3 × 3 transformation matrices $\boldsymbol{P}$ and $\boldsymbol{Q} = \boldsymbol{P}^{-1}$

For inverse transformations (against the arrow) replace $\boldsymbol{P}$ by $\boldsymbol{Q}$ and *vice versa.*

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ C \to A \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ A \to I \end{cases}$ Unique axis **b** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to C \end{cases}$ (Fig. 1.5.1.2*a*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ B \to I \end{cases}$ Unique axis **c** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to A \end{cases}$ (Fig. 1.5.1.2*b*)	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Cell choice 1 → cell choice 2: $\begin{cases} P \to P \\ B \to C \end{cases}$ Cell choice 2 → cell choice 3: $\begin{cases} P \to P \\ C \to I \end{cases}$ Unique axis **a** invariant Cell choice 3 → cell choice 1: $\begin{cases} P \to P \\ I \to B \end{cases}$ (Fig. 1.5.1.2*c*)	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **b** → unique axis **c** Cell choice 1: $\begin{cases} P \to P \\ C \to A \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **b** → unique axis **a** Cell choice 1: $\begin{cases} P \to P \\ C \to B \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ A \to C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
Unique axis **c** → unique axis **a** Cell choice 1: $\begin{cases} P \to P \\ A \to B \end{cases}$ Cell choice 2: $\begin{cases} P \to P \\ B \to C \end{cases}$ Cell choice invariant Cell choice 3: $\begin{cases} P \to P \\ I \to I \end{cases}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Monoclinic (*cf.* Sections 1.5.4.3 and 2.1.3.15)
$I \to P$ (Fig. 1.5.1.3)	$\begin{pmatrix} \bar{\frac{1}{2}} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \bar{\frac{1}{2}} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$	Orthorhombic Tetragonal Cubic
$F \to P$ (Fig. 1.5.1.4)	$\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$	Orthorhombic Tetragonal Cubic

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
$(\mathbf{b}, \mathbf{a}, \bar{\mathbf{c}}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{c}, \mathbf{a}, \mathbf{b}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\bar{\mathbf{c}}, \mathbf{b}, \mathbf{a}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{b}, \mathbf{c}, \mathbf{a}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$(\mathbf{a}, \bar{\mathbf{c}}, \mathbf{b}) \rightarrow (\mathbf{a}, \mathbf{b}, \mathbf{c})$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$	Unconventional orthorhombic setting
$P \rightarrow C_1$, $I \rightarrow F_1$ (Fig. 1.5.1.5), **c** axis invariant	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \bar{\frac{1}{2}} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 1.5.4.3)
$P \rightarrow C_2$, $I \rightarrow F_2$ (Fig. 1.5.1.5), **c** axis invariant	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{\frac{1}{2}} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Tetragonal (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_1, obverse setting (Fig. 1.5.1.6*a*,*c*)	$\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \bar{\frac{1}{3}} & \bar{\frac{1}{3}} \\ \frac{1}{3} & \frac{1}{3} & \bar{\frac{2}{3}} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_2, obverse setting (Fig. 1.5.1.6*c*)	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 1 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{3}} & \frac{2}{3} & \bar{\frac{1}{3}} \\ \bar{\frac{2}{3}} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_3, obverse setting (Fig. 1.5.1.6*c*)	$\begin{pmatrix} \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{3}} & \bar{\frac{1}{3}} & \frac{2}{3} \\ \frac{1}{3} & \bar{\frac{2}{3}} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_1, reverse setting (Fig. 1.5.1.6*d*)	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \\ 0 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{2}{3}} & \frac{1}{3} & \frac{1}{3} \\ \bar{\frac{1}{3}} & \bar{\frac{1}{3}} & \frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_2, reverse setting (Fig. 1.5.1.6*b*,*d*)	$\begin{pmatrix} 0 & 1 & 1 \\ \bar{1} & 0 & 1 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \bar{\frac{2}{3}} & \frac{1}{3} \\ \frac{2}{3} & \bar{\frac{1}{3}} & \bar{\frac{1}{3}} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ triple hexagonal cell R_3, reverse setting (Fig. 1.5.1.6*d*)	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \bar{\frac{2}{3}} \\ \bar{\frac{1}{3}} & \frac{2}{3} & \bar{\frac{1}{3}} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ orthohexagonal centred cell C_1 (Fig. 1.5.1.7)	$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{\frac{1}{2}} & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ orthohexagonal centred cell C_2 (Fig. 1.5.1.7)	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{\frac{1}{2}} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Hexagonal cell $P \rightarrow$ orthohexagonal centred cell C_3 (Fig. 1.5.1.7)	$\begin{pmatrix} 0 & \bar{2} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{2}} & 1 & 0 \\ \bar{\frac{1}{2}} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_1 (Fig. 1.5.1.8)	$\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \bar{\frac{1}{3}} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_2 (Fig. 1.5.1.8)	$\begin{pmatrix} 2 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 \\ \bar{\frac{1}{3}} & \frac{2}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple hexagonal cell H_3 (Fig. 1.5.1.8)	$\begin{pmatrix} 1 & \bar{2} & 0 \\ 2 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{3}} & \frac{2}{3} & 0 \\ \bar{\frac{2}{3}} & \frac{1}{3} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple rhombohedral cell D_1	$\begin{pmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{2}{3} & \bar{\frac{1}{3}} & \frac{1}{3} \\ \frac{1}{3} & \frac{2}{3} & \frac{1}{3} \\ \bar{\frac{1}{3}} & \bar{\frac{1}{3}} & \frac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Hexagonal cell $P \rightarrow$ triple rhombohedral cell D_2	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & \bar{1} & 1 \\ 1 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{2}{3}} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \bar{\frac{2}{3}} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$	Trigonal Hexagonal (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \frac{2}{3} & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ \bar{\frac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{3}{2} & 0 & 0 \\ \bar{\frac{1}{2}} & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \bar{\frac{1}{3}} & \bar{1} & 0 \\ \frac{1}{3} & \bar{1} & 0 \\ \bar{\frac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{3}{2}} & \frac{3}{2} & 0 \\ \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 0 \\ \bar{1} & 1 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 1.5.1.9*a*)	$\begin{pmatrix} \bar{\frac{1}{3}} & 1 & 0 \\ \bar{\frac{2}{3}} & 0 & 0 \\ \bar{\frac{2}{3}} & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{\frac{3}{2}} & 0 \\ 1 & \bar{\frac{1}{2}} & 0 \\ 0 & \bar{1} & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \frac{2}{3} & 0 \\ 0 & \frac{1}{3} & 1 \\ 1 & \bar{\frac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 1 \\ \frac{3}{2} & 0 & 0 \\ \bar{\frac{1}{2}} & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \bar{\frac{1}{3}} & \bar{1} \\ 0 & \frac{1}{3} & \bar{1} \\ 1 & \bar{\frac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \bar{\frac{3}{2}} & \frac{3}{2} & 0 \\ \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Triple hexagonal cell R, obverse setting $\rightarrow$ A-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 1.5.1.9*b*)	$\begin{pmatrix} 0 & \bar{\frac{1}{3}} & 1 \\ 0 & \bar{\frac{2}{3}} & 0 \\ 1 & \bar{\frac{2}{3}} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 1 \\ 0 & \bar{\frac{3}{2}} & 0 \\ 1 & \bar{\frac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 1 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{\frac{1}{2}} & \bar{\frac{1}{2}} \\ 0 & \frac{1}{2} & \bar{\frac{1}{2}} \\ 1 & 0 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell $\rightarrow$ C-centred monoclinic cell, unique axis **b**, cell choice 2 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \\ \bar{1} & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{2}} & 1 & \bar{\frac{1}{2}} \\ \bar{\frac{1}{2}} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)

Table 1.5.1.1 (continued)

Transformation	$\boldsymbol{P}$	$\boldsymbol{Q} = \boldsymbol{P}^{-1}$	Crystal system
Primitive rhombohedral cell → *C*-centred monoclinic cell, unique axis **b**, cell choice 3 (Fig. 1.5.1.10*a*)	$\begin{pmatrix} \bar{1} & 1 & 1 \\ \bar{1} & \bar{1} & 1 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 1 (Fig.1.5.1.10*b*)	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{\frac{1}{2}} & \bar{\frac{1}{2}} \\ 0 & \frac{1}{2} & \bar{\frac{1}{2}} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 2 (Fig. 1.5.1.10*b*)	$\begin{pmatrix} 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \\ 1 & \bar{1} & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ \bar{\frac{1}{2}} & 1 & \bar{\frac{1}{2}} \\ \bar{\frac{1}{2}} & 0 & \frac{1}{2} \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)
Primitive rhombohedral cell → *A*-centred monoclinic cell, unique axis **c**, cell choice 3 (Fig. 1.5.1.10*b*)	$\begin{pmatrix} 1 & \bar{1} & 1 \\ 1 & \bar{1} & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{\frac{1}{2}} & \bar{\frac{1}{2}} & 1 \\ \frac{1}{2} & \bar{\frac{1}{2}} & 0 \end{pmatrix}$	Rhombohedral space groups (*cf.* Section 1.5.4.3)

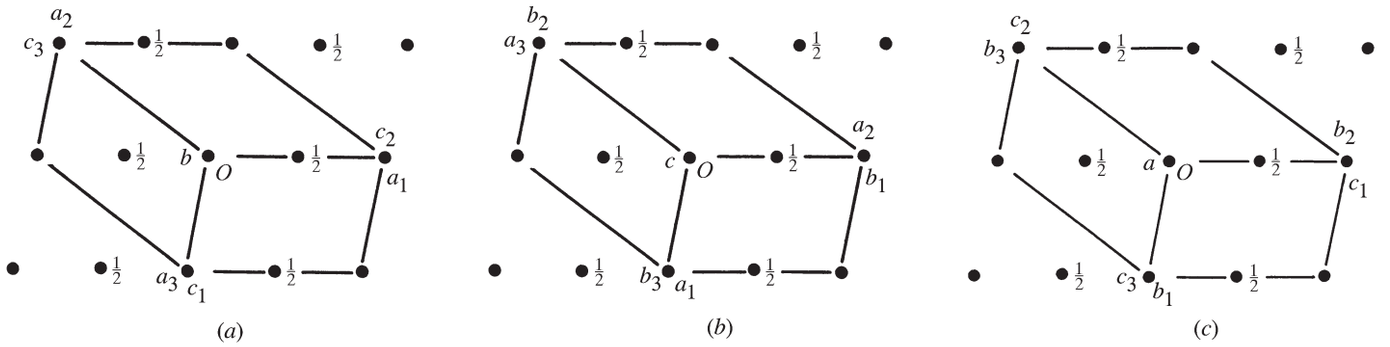


Figure 1.5.1.2
Monoclinic centred lattice, projected along the unique axis. The origin for all the cells is the same. The fractions $\frac{1}{2}$ indicate the height of the lattice points along the axis of projection.

(*a*) Unique axis *b*:
Cell choice 1: *C*-centred cell a_1, b, c_1.
Cell choice 2: *A*-centred cell a_2, b, c_2.
Cell choice 3: *I*-centred cell a_3, b, c_3.

(*b*) Unique axis *c*:
Cell choice 1: *A*-centred cell a_1, b_1, c.
Cell choice 2: *B*-centred cell a_2, b_2, c.
Cell choice 3: *I*-centred cell a_3, b_3, c.

(*c*) Unique axis *a*:
Cell choice 1: *B*-centred cell a, b_1, c_1.
Cell choice 2: *C*-centred cell a, b_2, c_2.
Cell choice 3: *I*-centred cell a, b_3, c_3.

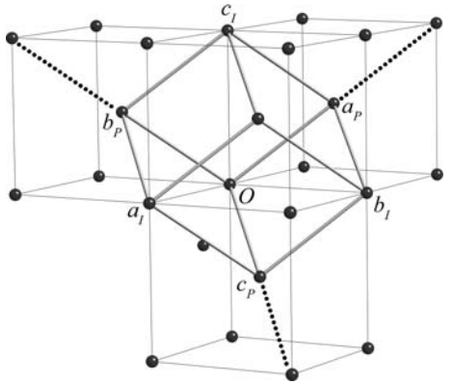


Figure 1.5.1.3
Body-centred cell *I* with a_I, b_I, c_I and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *I* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{3}$ and $\alpha = 109.47^\circ$ (rhombohedral axes) or a triple hexagonal cell with $a_{\rm hex} = a_c\sqrt{2}$ and $c_{\rm hex} = a_c \frac{1}{2}\sqrt{3}$ (hexagonal axes).

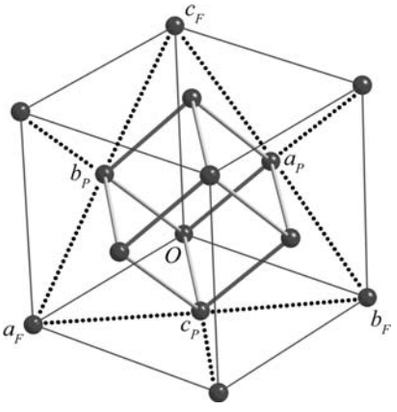


Figure 1.5.1.4
Face-centred cell *F* with a_F, b_F, c_F and a corresponding primitive cell *P* with a_P, b_P, c_P. The origin for both cells is *O*. A cubic *F* cell with lattice constant a_c can be considered as a primitive rhombohedral cell with $a_{\rm rh} = a_c \frac{1}{2}\sqrt{2}$ and $\alpha = 60^\circ$ (rhombohedral axes) or a triple hexagonal cell with $a_{\rm hex} = a_c \frac{1}{2}\sqrt{2}$ and $c_{\rm hex} = a_c\sqrt{3}$ (hexagonal axes).

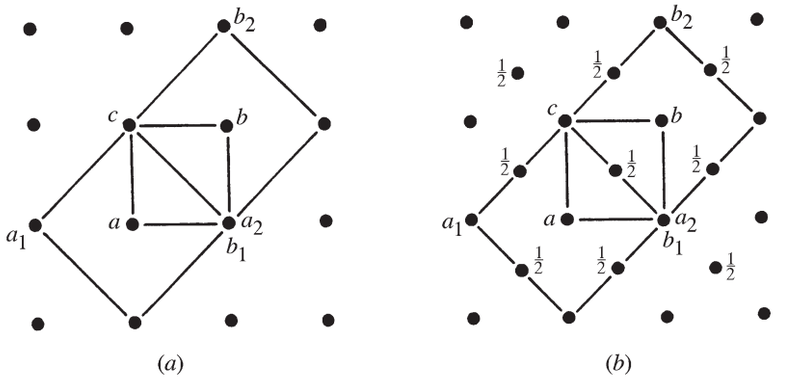


Figure 1.5.1.5
Tetragonal lattices, projected along $[00\bar{1}]$. (*a*) Primitive cell P with a, b, c and the C-centred cells C_1 with a_1, b_1, c and C_2 with a_2, b_2, c. The origin for all three cells is the same. (*b*) Body-centred cell I with a, b, c and the F-centred cells F_1 with a_1, b_1, c and F_2 with a_2, b_2, c. The origin for all three cells is the same. The fractions $\frac{1}{2}$ indicate the height of the lattice points along the axis of projection.

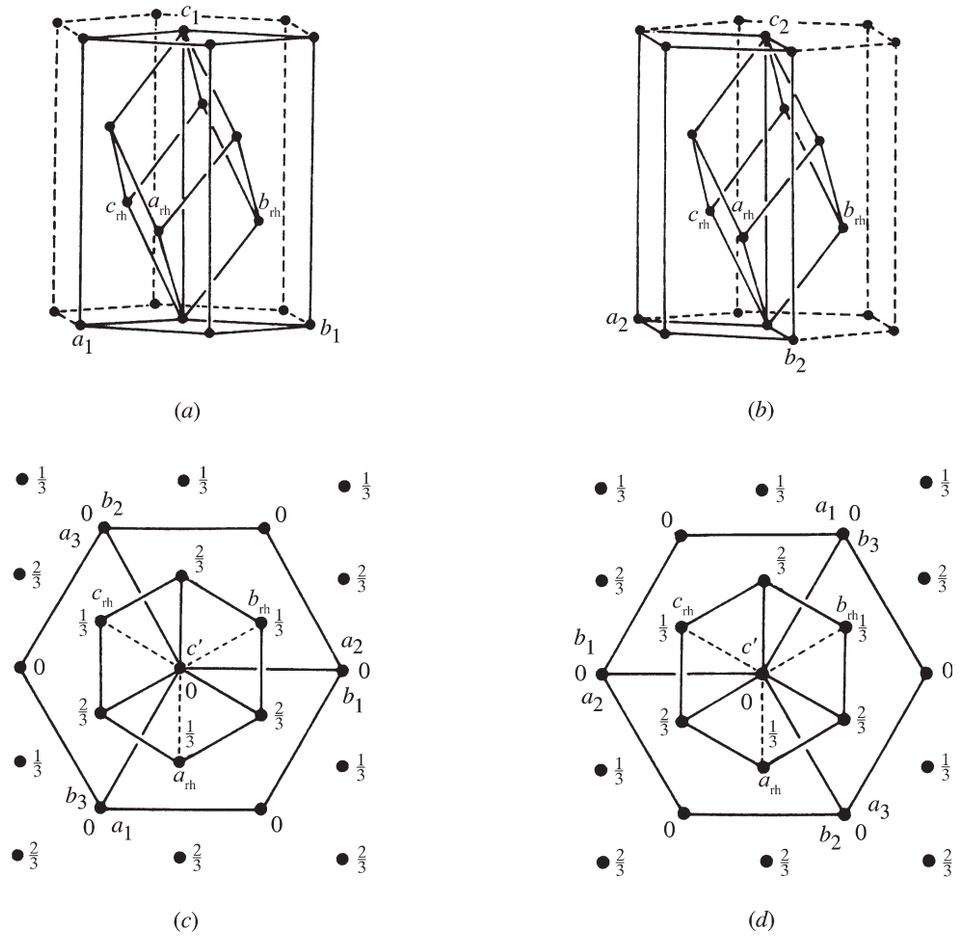


Figure 1.5.1.6
Unit cells in the rhombohedral lattice: same origin for all cells. The basis of the rhombohedral cell is labelled a_{rh}, b_{rh}, c_{rh}. Two settings of the triple hexagonal cell are possible with respect to a primitive rhombohedral cell: The *obverse setting* with the lattice points 0, 0, 0; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ has been used in *International Tables* since 1952. Its general reflection condition is $-h + k + l = 3n$. The *reverse setting* with lattice points 0, 0, 0; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$ was used in the 1935 edition. Its general reflection condition is $h - k + l = 3n$. The fractions indicate the height of the lattice points along the axis of projection. (*a*) Obverse setting of triple hexagonal cell a_1, b_1, c_1 in relation to the primitive rhombohedral cell a_{rh}, b_{rh}, c_{rh}. (*b*) Reverse setting of triple hexagonal cell a_2, b_2, c_2 in relation to the primitive rhombohedral cell a_{rh}, b_{rh}, c_{rh}. (*c*) Primitive rhombohedral cell (- - - lower edges), a_{rh}, b_{rh}, c_{rh} in relation to the three triple hexagonal cells in obverse setting a_1, b_1, c'; a_2, b_2, c'; a_3, b_3, c'. Projection along c'. (*d*) Primitive rhombohedral cell (- - - lower edges), a_{rh}, b_{rh}, c_{rh} in relation to the three triple hexagonal cells in reverse setting a_1, b_1, c'; a_2, b_2, c'; a_3, b_3, c'. Projection along c'.

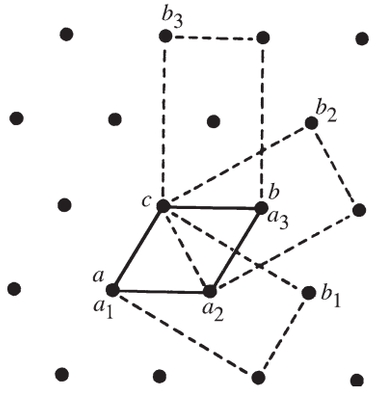


Figure 1.5.1.7
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three C-centred (orthohexagonal) cells a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.

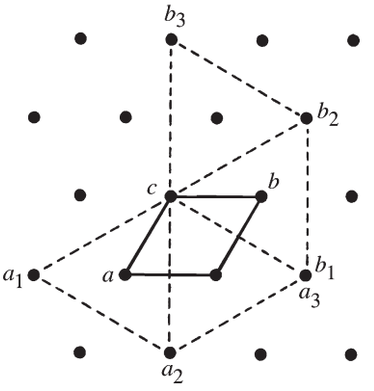
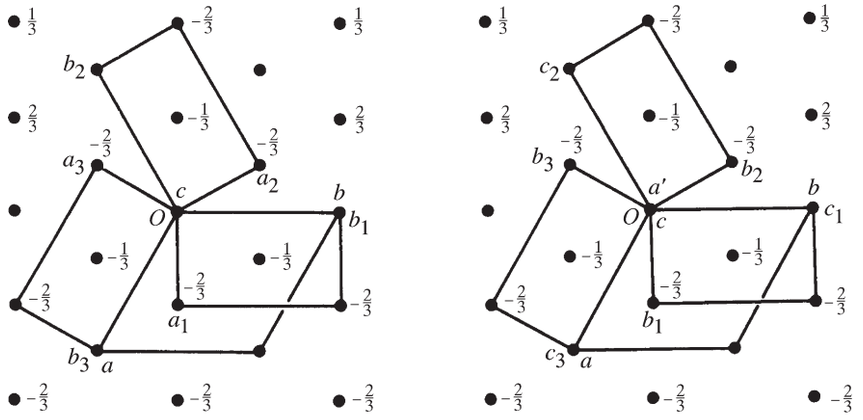
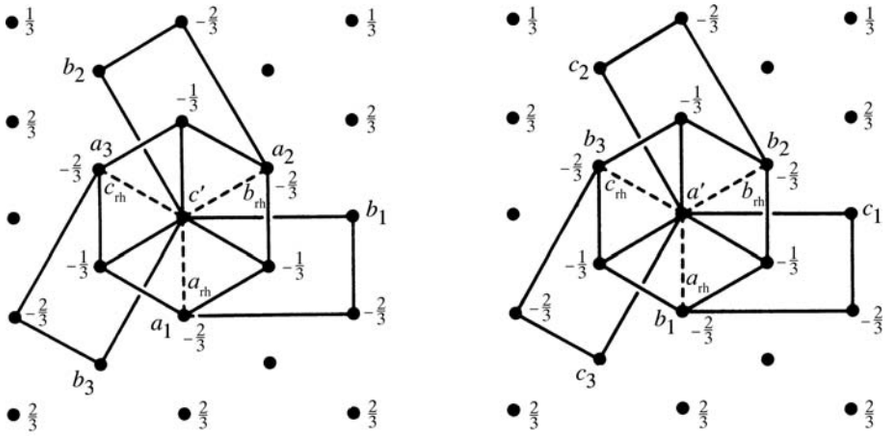


Figure 1.5.1.8
Hexagonal lattice projected along $[00\bar{1}]$. Primitive hexagonal cell P with a, b, c and the three triple hexagonal cells H with a_1, b_1, c; a_2, b_2, c; a_3, b_3, c. The origin for all cells is the same.



(*a*) (*b*)

Figure 1.5.1.9
Rhombohedral lattice with a triple hexagonal unit cell a, b, c in obverse setting (*i.e.* unit cell a_1, b_1, c in Fig. 1.5.1.6*c*) and the three centred monoclinic cells. (*a*) C-centred cells C_1 with a_1, b_1, c; C_2 with a_2, b_2, c; and C_3 with a_3, b_3, c. The unique monoclinic axes are b_1, b_2 and b_3, respectively. The origin for all four cells is the same. (*b*) A-centred cells A_1 with a', b_1, c_1; A_2 with a', b_2, c_2; and A_3 with a', b_3, c_3. The unique monoclinic axes are c_1, c_2 and c_3, respectively. The origin for all four cells is the same. The fractions indicate the height of the lattice points along the axis of projection.



(*a*) (*b*)

Figure 1.5.1.10
Rhombohedral lattice with primitive rhombohedral cell a_{rh}, b_{rh}, c_{rh} and the three centred monoclinic cells. (*a*) C-centred cells C_1 with a_1, b_1, c'; C_2 with a_2, b_2, c'; and C_3 with a_3, b_3, c'. The unique monoclinic axes are b_1, b_2 and b_3, respectively. The origin for all four cells is the same. (*b*) A-centred cells A_1 with a', b_1, c_1; A_2 with a', b_2, c_2; and A_3 with a', b_3, c_3. The unique monoclinic axes are c_1, c_2 and c_3, respectively. The origin for all four cells is the same. The fractions indicate the height of the lattice points along the axis of projection.

$$\begin{pmatrix} x_P \\ y_P \\ z_P \end{pmatrix} = \boldsymbol{P}^{-1}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}\begin{pmatrix} x_F \\ y_F \\ z_F \end{pmatrix} = \begin{pmatrix} -x_F + y_F + z_F \\ x_F - y_F + z_F \\ x_F + y_F - z_F \end{pmatrix}.$$

For example, the coordinates $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_F$ of the end point of $\mathbf{a}_F$ with respect to the conventional basis become $\begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}_P$ in the primitive basis, the centring point $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}_F$ of the $\mathbf{a}_F, \mathbf{b}_F$ plane becomes the end point $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_P$ of $\mathbf{c}_P$ *etc.*

The concise notation of the transformation matrices is widely used in the tables of maximal subgroups of space groups in *International Tables for Crystallography* Volume A1 (2010), where $(\boldsymbol{P}, \boldsymbol{p})$ describes the relation between the conventional bases of a group and its maximal subgroups. For example, the expression $(\boldsymbol{P}, \boldsymbol{p}) = (\mathbf{a} - \mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}; 0, 0, \frac{1}{2})$ (*cf.* the table of maximal subgroups of $P\bar{4}2m$, No. 111, in Volume A1) stands for

$$\boldsymbol{P} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \text{ and } \boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}.$$

Note that the matrix elements of $\boldsymbol{P}$ in equation (1.5.1.8) are read by *columns* since they act on the *row* matrices of basis vectors, and not by *rows*, as in the shorthand notation of symmetry operations which apply to *column* matrices of coordinates (*cf.* Section 1.2.2.1).

1.5.1.3. General change of coordinate system

A general change of the coordinate system involves both an origin shift and a change of the basis. Such a transformation of the coordinate system is described by the matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$, where the (3×3) matrix $\boldsymbol{P}$ relates the new basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ to the old one $\mathbf{a}, \mathbf{b}, \mathbf{c}$ according to equation (1.5.1.4). The origin shift is described by the *shift vector* $\mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}$. The coordinates of the new origin O' with respect to the old coordinate system $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are given by the (3×1) column $\boldsymbol{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$.

The general coordinate transformation can be performed in two consecutive steps. Because the origin shift $\boldsymbol{p}$ refers to the old basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$, it has to be applied first (as described in Section 1.5.1.1), followed by the change of the basis (*cf.* Section 1.5.1.2):

$$\boldsymbol{x}' = (\boldsymbol{P}, \boldsymbol{o})^{-1}(\boldsymbol{I}, \boldsymbol{p})^{-1}\boldsymbol{x} = ((\boldsymbol{I}, \boldsymbol{p})(\boldsymbol{P}, \boldsymbol{o}))^{-1}\boldsymbol{x} = (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x}. \quad (1.5.1.6)$$

Here, $\boldsymbol{I}$ is the three-dimensional unit matrix and $\boldsymbol{o}$ is the (3×1) column matrix containing only zeros as coefficients.

The formulae for the change of the *point coordinates* from $\boldsymbol{x}$ to $\boldsymbol{x}'$ uses $(\boldsymbol{Q}, \ \boldsymbol{q}) = (\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{P}^{-1}, \ -\boldsymbol{P}^{-1}\boldsymbol{p})$, *i.e.*

$$\begin{pmatrix} x_1' \\ x_2' \\ x_3' \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}$$

with $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ and $\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$,

thus $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p})$. (1.5.1.7)

The effect of a general change of the coordinate system $(\boldsymbol{P}, \boldsymbol{p})$ on the coefficients of a vector $\mathbf{r}$ is reduced to the linear transformation described by $\boldsymbol{P}$, as the vector coefficients are not affected by the origin shift [*cf.* equation (1.5.1.3)].

Hereafter, the data for the matrix–column pair

$$(\boldsymbol{P}, \boldsymbol{p}) = \left(\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}, \ \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}\right)$$

are often written in the following concise form:

$$P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, \ \ P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, \ \ P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}; \ \ p_1, p_2, p_3. \quad (1.5.1.8)$$

1.5.2. Transformations of crystallographic quantities under coordinate transformations

By H. Wondratschek and M. I. Aroyo

1.5.2.1. Covariant and contravariant quantities

If the *direct* or *crystal* basis is transformed by the transformation matrix $\boldsymbol{P}$: $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$, the corresponding basis vectors of the *reciprocal (or dual) basis* transform as (*cf.* Section 1.3.2.5)

$$\begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}, \quad (1.5.2.1)$$

where the notation $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ is applied (*cf.* Section 1.5.1.2).

The quantities that transform in the same way as the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ are called *covariant* with respect to the basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and *contravariant* with respect to the reciprocal basis $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$. Such quantities are the *Miller indices* (hkl) of a plane (or a set of planes) in direct space and the vector coefficients (h, k, l) of the vector perpendicular to those planes, referred to the reciprocal basis $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$:

$$(h', k', l') = (h, k, l)\boldsymbol{P}. \quad (1.5.2.2)$$

Quantities like the vector coefficients of any vector $\boldsymbol{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}$ in direct space (or the *indices of a direction* in direct space) are covariant with respect to the basis vectors $\begin{pmatrix} \mathbf{a}^* \\ \mathbf{b}^* \\ \mathbf{c}^* \end{pmatrix}$ and contravariant with respect to $\mathbf{a}, \mathbf{b}, \mathbf{c}$:

$$\begin{pmatrix} u' \\ v' \\ w' \end{pmatrix} = \boldsymbol{Q}\begin{pmatrix} u \\ v \\ w \end{pmatrix}. \quad (1.5.2.3)$$

1.5.2.2. Metric tensors of direct and reciprocal lattices

The metric tensor of a crystal lattice with a basis **a**, **b**, **c** is the (3 × 3) matrix

$$\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix},$$

which can formally be described as

$$\boldsymbol{G} = (\mathbf{a},\mathbf{b},\mathbf{c})^T\cdot(\mathbf{a},\mathbf{b},\mathbf{c}) = \begin{pmatrix}\mathbf{a}\\ \mathbf{b}\\ \mathbf{c}\end{pmatrix}\cdot(\mathbf{a},\mathbf{b},\mathbf{c})$$

(*cf.* Section 1.3.2). The transformation of the metric tensor under the coordinate transformation $(\boldsymbol{P},\boldsymbol{p})$ follows directly from its definition:

$$\begin{aligned}\boldsymbol{G}' &= (\mathbf{a}',\mathbf{b}',\mathbf{c}')^T\cdot(\mathbf{a}',\mathbf{b}',\mathbf{c}') = [(\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P}]^T\cdot(\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P}\\ &= \boldsymbol{P}^T(\mathbf{a},\mathbf{b},\mathbf{c})^T\cdot(\mathbf{a},\mathbf{b},\mathbf{c})\boldsymbol{P} = \boldsymbol{P}^T\boldsymbol{G}\boldsymbol{P},\end{aligned} \tag{1.5.2.4}$$

where $\boldsymbol{P}^T$ is the transposed matrix of $\boldsymbol{P}$. The transformation behaviour of $\boldsymbol{G}$ under $(\boldsymbol{P},\boldsymbol{p})$ is determined by the matrix $\boldsymbol{P}$, *i.e.* $\boldsymbol{G}$ is not affected by an origin shift $\boldsymbol{p}$.

The volume V of the unit cell defined by the basis vectors **a**, **b**, **c** can be obtained from the determinant of the metric tensor, $V^2 = \det(\boldsymbol{G})$. The transformation behaviour of V under a coordinate transformation follows from the transformation behaviour of the metric tensor [note that $\det(\boldsymbol{P}) = \det(\boldsymbol{P}^T)$]: $(V')^2 = \det(\boldsymbol{G}') = \det(\boldsymbol{P}^T\boldsymbol{G}\boldsymbol{P}) = \det(\boldsymbol{P})\det(\boldsymbol{P}^T)\det(\boldsymbol{G}) = \det(\boldsymbol{P})^2V^2$, *i.e.*

$$V' = |\det(\boldsymbol{P})|V, \tag{1.5.2.5}$$

which is reduced to $V' = \det(\boldsymbol{P})V$ if $\det(\boldsymbol{P}) > 0$.

Similarly, the metric tensor $\boldsymbol{G}^*$ of the reciprocal lattice and the volume V^* of the unit cell defined by the basis vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ transform as

$$\boldsymbol{G}^{*\prime} = \boldsymbol{Q}\boldsymbol{G}^*\boldsymbol{Q}^T, \tag{1.5.2.6}$$

$$V^{*\prime} = |\det(\boldsymbol{Q})|V^* \text{ or } V^{*\prime} = \det(\boldsymbol{Q})V^* = [1/\det(\boldsymbol{P})]V^* \text{ if } \det(\boldsymbol{Q}) > 0. \tag{1.5.2.7}$$

Again, it is only the linear part $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ that determines the transformation behaviour of $\boldsymbol{G}^*$ and V^* under coordinate transformations.

1.5.2.3. Transformation of matrix–column pairs of symmetry operations

The *matrix–column pairs for the symmetry operations* are changed by a change of the coordinate system (see Section 1.2.2 for details of the matrix description of symmetry operations). A symmetry operation W that maps a point X to an image point $\tilde{X}$ is described in the 'old' (unprimed) coordinate system by the system of equations

$$\begin{aligned}\tilde{x_1} &= W_{11}x_1 + W_{12}x_2 + W_{13}x_3 + w_1\\ \tilde{x_2} &= W_{21}x_1 + W_{22}x_2 + W_{23}x_3 + w_2\\ \tilde{x_3} &= W_{31}x_1 + W_{32}x_2 + W_{33}x_3 + w_3,\end{aligned} \tag{1.5.2.8}$$

i.e. by the matrix–column pair $(\boldsymbol{W},\boldsymbol{w})$:

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} = (\boldsymbol{W},\boldsymbol{w})\boldsymbol{x}. \tag{1.5.2.9}$$

In the new (primed) coordinate system, the symmetry operation W is described by the pair $(\boldsymbol{W}',\boldsymbol{w}')$:

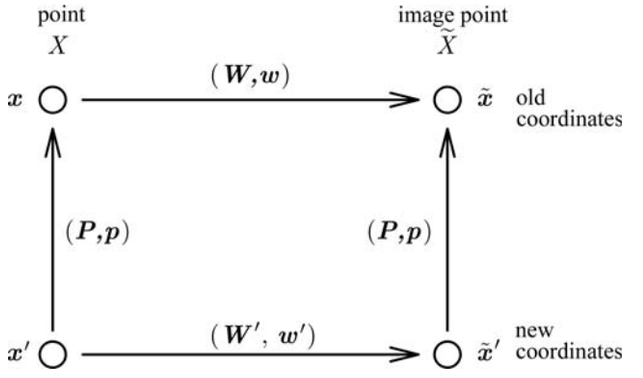


Figure 1.5.2.1
Illustration of the transformation of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$, also called a 'mapping of mappings'.

$$\tilde{\boldsymbol{x}}' = (\boldsymbol{W}',\boldsymbol{w}')\boldsymbol{x}' = \boldsymbol{W}'\boldsymbol{x}' + \boldsymbol{w}'. \tag{1.5.2.10}$$

The relation between $(\boldsymbol{W},\boldsymbol{w})$ and $(\boldsymbol{W}',\boldsymbol{w}')$ is derived *via* the transformation matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$, which specifies the change of the coordinate system. The successive application of equations (1.5.1.7), (1.5.2.9) and again (1.5.1.7) results in $\tilde{\boldsymbol{x}}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$, which compared with equation (1.5.2.10) gives

$$(\boldsymbol{W}',\boldsymbol{w}') = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}). \tag{1.5.2.11}$$

The result indicates that the change of the matrix–column pairs of symmetry operations $(\boldsymbol{W},\boldsymbol{w})$ under a coordinate transformation described by the matrix–column pair $(\boldsymbol{P},\boldsymbol{p})$ is realized by the conjugation of $(\boldsymbol{W},\boldsymbol{w})$ by $(\boldsymbol{P},\boldsymbol{p})$. The multiplication of the matrix–column pairs on the *right-hand side* of equation (1.5.2.11), namely $(\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1},-\boldsymbol{P}^{-1}\boldsymbol{p})(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1}\boldsymbol{W},\boldsymbol{P}^{-1}\boldsymbol{w}-\boldsymbol{P}^{-1}\boldsymbol{p})(\boldsymbol{P},\boldsymbol{p}) = (\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P},\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{p}+\boldsymbol{P}^{-1}\boldsymbol{w}-\boldsymbol{P}^{-1}\boldsymbol{p})$, results in the factorization of the relation (1.5.2.11) into a pair of equations for the rotation and translation parts of $(\boldsymbol{W}',\boldsymbol{w}')$:

$$\boldsymbol{W}' = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} = \boldsymbol{Q}\boldsymbol{W}\boldsymbol{P} \tag{1.5.2.12}$$

and

$$\begin{aligned}\boldsymbol{w}' &= \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{p} + \boldsymbol{P}^{-1}\boldsymbol{w} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{w} + \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p})\\ &= \boldsymbol{Q}(\boldsymbol{w} + \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p}) = \boldsymbol{Q}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}).\end{aligned} \tag{1.5.2.13}$$

The whole formalism described above can be visualized by means of an instructive diagram, Fig. 1.5.2.1, displaying the transformation of the matrix–column pairs of symmetry operations under coordinate transformations, the so-called *mapping of mappings*.

The points X (left) and $\tilde{X}$ (right), and the corresponding columns of coordinates $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$, and $\boldsymbol{x}'$ and $\tilde{\boldsymbol{x}}'$, are referred to the old and to the new coordinate systems, respectively. The transformation matrices of each step are indicated next to the edges of the diagram, while the arrows indicate the direction, *e.g.* $\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$ but $\boldsymbol{x}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\boldsymbol{x}$. From $\boldsymbol{x}'$ to $\tilde{\boldsymbol{x}}'$ it is possible to proceed in two different ways:
(i) $\tilde{\boldsymbol{x}}' = (\boldsymbol{W}',\boldsymbol{w}')\boldsymbol{x}'$,
(ii) $\tilde{\boldsymbol{x}}' = (\boldsymbol{P},\boldsymbol{p})^{-1}\tilde{\boldsymbol{x}} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})\boldsymbol{x} = (\boldsymbol{P},\boldsymbol{p})^{-1}(\boldsymbol{W},\boldsymbol{w})(\boldsymbol{P},\boldsymbol{p})\boldsymbol{x}'$.
The comparison of (i) and (ii) yields equation (1.5.2.11).

1.5.2.4. Augmented-matrix formalism

The augmented-matrix formalism (*cf.* Section 1.2.2) simplifies the equations of the coordinate transformations discussed above.

The matrices $\boldsymbol{P}$, $\boldsymbol{Q}$ may be combined with the corresponding columns $\boldsymbol{p}$, $\boldsymbol{q}$ to form (4×4) matrices:

$$\mathbb{P} = \left(\begin{array}{c|c} \boldsymbol{P} & \boldsymbol{p} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{Q} = \mathbb{P}^{-1} = \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \qquad (1.5.2.14)$$

where $\boldsymbol{0}$ is a 1×3 row with zero coefficients. As already indicated in Section 1.2.2, the horizontal and vertical lines in the augmented matrices have no mathematical meaning; they serve as guide to the eye so that the coefficients can be recognized more easily.

Analogously, the (3×1) columns $\boldsymbol{x}$ and $\boldsymbol{x}'$ are augmented to (4×1) columns by adding '1' as fourth coordinate in order to enable matrix multiplication with the augmented matrices: $\mathbb{x} = \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix}$; $\mathbb{x}' = \begin{pmatrix} x'_1 \\ x'_2 \\ \underline{x'_3} \\ 1 \end{pmatrix}$. Using the augmented matrices, the transformation behaviour of point coordinates [*cf.* equation (1.5.1.7)] takes the form

$$\begin{aligned} \mathbb{x}' = \mathbb{P}^{-1}\mathbb{x} = \mathbb{Q}\mathbb{x} &= \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix} \\ &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} x_1 \\ x_2 \\ \underline{x_3} \\ 1 \end{pmatrix} \\ &= \begin{pmatrix} Q_{11}x_1 + Q_{12}x_2 + Q_{13}x_3 + q_1 \\ Q_{21}x_1 + Q_{22}x_2 + Q_{23}x_3 + q_2 \\ \underline{Q_{31}x_1 + Q_{32}x_2 + Q_{33}x_3 + q_3} \\ 1 \end{pmatrix}. \end{aligned} \qquad (1.5.2.15)$$

The difference in the transformation behaviour of point coordinates and vector coefficients under coordinate transformations becomes obvious if the augmented-matrix formalism is applied. The (3×1) column of coefficients of a vector between points X and Y,

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ y_3 - x_3 \end{pmatrix},$$

is augmented by adding *zero* as fourth coefficient:

$$\mathbb{r} = \mathbb{y} - \mathbb{x} = \begin{pmatrix} y_1 - x_1 \\ y_2 - x_2 \\ \underline{y_3 - x_3} \\ 0 \end{pmatrix},$$

and this specific form of $\mathbb{r}$ reflects its specific transformation properties, namely that it is unaffected by origin shifts:

$$\begin{aligned} \mathbb{r}' = \mathbb{P}^{-1}\mathbb{r} = \mathbb{Q}\mathbb{r} &= \left(\begin{array}{c|c} \boldsymbol{Q} & \boldsymbol{q} \\ \hline \boldsymbol{0} & 1 \end{array}\right) \begin{pmatrix} r_1 \\ r_2 \\ \underline{r_3} \\ 0 \end{pmatrix} \\ &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} r_1 \\ r_2 \\ \underline{r_3} \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} Q_{11}r_1 + Q_{12}r_2 + Q_{13}r_3 \\ Q_{21}r_1 + Q_{22}r_2 + Q_{23}r_3 \\ \underline{Q_{31}r_1 + Q_{32}r_2 + Q_{33}r_3} \\ 0 \end{pmatrix}. \end{aligned} \qquad (1.5.2.16)$$

The Miller indices (hkl) are coefficients of vectors in reciprocal space (plane normals). Therefore, the (1×3) rows (hkl) are augmented by 0: $(hkl|0)$. Thus, only the linear part $\boldsymbol{P}$ of the general coordinate transformation $(\boldsymbol{P}, \boldsymbol{p})$ acts on the Miller indices while the origin shift has no effect, *cf.* equation (1.5.2.2).

The augmented-matrix formulation of transformation of symmetry operations (1.5.2.11) is straightforward if the matrices $\boldsymbol{W}$ and $\boldsymbol{W}'$ are combined with the corresponding columns $\boldsymbol{w}$ and $\boldsymbol{w}'$ to form (4×4) matrices:

$$\mathbb{W} = \left(\begin{array}{c|c} \boldsymbol{W} & \boldsymbol{w} \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{W}' = \left(\begin{array}{c|c} \boldsymbol{W}' & \boldsymbol{w}' \\ \hline \boldsymbol{0} & 1 \end{array}\right) = \left(\begin{array}{ccc|c} W'_{11} & W'_{12} & W'_{13} & w'_1 \\ W'_{21} & W'_{22} & W'_{23} & w'_2 \\ W'_{31} & W'_{32} & W'_{33} & w'_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

Thus, equation (1.5.2.11) is replaced by its (4×4) analogue:

$$\begin{aligned} \mathbb{W}' = \mathbb{P}^{-1}\mathbb{W}\mathbb{P} = \mathbb{Q}\mathbb{W}\mathbb{P} &= \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \cdot \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \\ &\cdot \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right), \end{aligned} \qquad (1.5.2.17)$$

where $\mathbb{P}$ and $\mathbb{Q}$ are defined according to equation (1.5.2.14). [Note that to avoid any confusion that might result from equation (1.5.2.17) being displayed over more than one line, the matrix multiplication is explicitly indicated by centred dots between the matrices.] In analogy to equation (1.5.2.11), the change of the augmented matrices of symmetry operations $\mathbb{W}$ under coordinate transformations represented by the augmented matrices $\mathbb{P}$ is described by the conjugation of $\mathbb{W}$ with $\mathbb{P}$.

The transformation behaviour of the vector coefficients becomes apparent if the (distance) vector $\mathbf{v}$ is treated as a

translation vector and the transformation behaviour of the translation is considered. The corresponding translation is then described by $(\boldsymbol{I}, \boldsymbol{v})$, *i.e.* $\boldsymbol{W} = \boldsymbol{I}$, $\boldsymbol{w} = \boldsymbol{v}$. Equation (1.5.2.13) shows that the translation and thus the translation vector are not changed under an origin shift, $(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{I}, \boldsymbol{p})$, because $(\boldsymbol{I}, \boldsymbol{v})' = (\boldsymbol{I}, \boldsymbol{v})$ holds. For the same reason, under a general coordinate transformation the origin shift has no effect on the vector coefficients, *cf.* equation (1.5.2.16).

1.5.2.5. Example: paraelectric-to-ferroelectric phase transition of GeTe

Coordinate transformations are essential in the study of structural relationships between crystal structures. Consider as an example two phases **A** (*basic* or *parent* structure) and **B** (*derivative* structure) of the same compound. Let the space group $\mathcal{H}$ of **B** be a proper subgroup of the space group $\mathcal{G}$ of **A**, $\mathcal{H} < \mathcal{G}$. The relationship between the two structures is characterized by a global distortion that, in general, can be decomposed into a homogeneous strain describing the distortion of the lattice of **B** relative to that of **A** and an atomic displacement field representing the displacements of the atoms of **B** from their positions in **A**. In order to facilitate the comparison of the two structures, first the coordinate system of structure **A** is transformed by an appropriate transformation $(\boldsymbol{P}, \boldsymbol{p})$ to that of structure **B**. This new description of **A** will be called the *reference description* of structure **A** relative to structure **B**. Now, the metric tensors $\boldsymbol{G}_{\mathbf{A}}$ of the reference description of **A** and $\boldsymbol{G}_{\mathbf{B}}$ are of the same type and are distinguished only by the values of their parameters. The adaptation of structure **A** to structure **B** can be performed in two further steps. In the first step the parameter values of $\boldsymbol{G}_{\mathbf{A}}$ are adapted to those of $\boldsymbol{G}_{\mathbf{B}}$ by an affine transformation which determines the metric deformation (spontaneous strain) of structure **B** relative to structure **A**. The result is a hypothetical structure which still differs from structure **B** by atomic displacements. In the second step these displacements are balanced out by shifting the individual atoms to those of structure **B**. In other words, if $\mathbf{a}, \mathbf{b}, \mathbf{c}$ represents the basis of the parent phase, then its image under the transformation $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}$ should be similar to the basis of the derivative phase $\mathbf{a}_{\mathcal{H}}, \mathbf{b}_{\mathcal{H}}, \mathbf{c}_{\mathcal{H}}$. The difference between $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ and $\mathbf{a}_{\mathcal{H}}, \mathbf{b}_{\mathcal{H}}, \mathbf{c}_{\mathcal{H}}$ determines the metric deformation (spontaneous strain) accompanying the transition between the two phases. Similarly, the differences between the images X' of the atomic positions X of the basic structure under the transformation $(\boldsymbol{P}, \boldsymbol{p})$ and the atomic positions $X_{\mathcal{H}}$ of the derivative structure give the atomic displacements that occur during the phase transition.

As an example we will consider the structural phase transition of GeTe, which is of displacive type, *i.e.* the phase transition is accomplished through small atomic displacements. The room-temperature ferroelectric phase belongs to the rhombohedral space group *R*3*m* (160). At about 720 K a structural phase transition takes place to a high-symmetry paraelectric cubic phase of the NaCl type. The following descriptions of the two phases of GeTe are taken from the ICSD:

(*a*) Wiedemeier & Siemers (1989), ICSD No. 56037. The symmetry of the high-temperature phase is described by the space group $Fm\bar{3}m$ (225) with cell parameters a_c = 6.009 Å and atomic coordinates listed as
Ge: 4*a* 0, 0, 0
Te: 4*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

(*b*) Chattopadhyay *et al.* (1987), ICSD No. 56038. The structure is described with respect to the hexagonal-axes setting of *R*3*m* (160) (*cf.* Section 1.5.3.1) with cell parameters $a_{\rm hex}$ = 4.164 (2) Å, $c_{\rm hex}$ = 10.69 (4) Å. The coordinates of the atoms in the asymmetric unit are given as
Ge: 3*a* 0, 0, 0.2376
Te: 3*a* 0, 0, 0.7624

The relation between the basis $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ of the *F*-centred cubic lattice and the basis $\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c$ of the reference description can be obtained by inspection. The $\mathbf{c}'_c$ axis of the reference hexagonal basis must be one of the cubic threefold axes, say [111]. The axes $\mathbf{a}'_c$ and $\mathbf{b}'_c$ must be lattice vectors of the *F*-centred lattice, perpendicular to the rhombohedral axis. They must have equal length, form an angle of 120°, and together with $\mathbf{c}'_c$ define a right-handed basis. For example, the vectors $\mathbf{a}'_c = \frac{1}{2}(-\mathbf{a}_c + \mathbf{b}_c)$, $\mathbf{b}'_c = \frac{1}{2}(-\mathbf{b}_c + \mathbf{c}_c)$ fulfil these conditions.

The transformation matrix $\boldsymbol{P}$ between the bases $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ and $\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c$ can also be derived from the data listed in Table 1.5.1.1 in two steps:

(i) A cubic *F* cell can be considered as a primitive rhombohedral cell with $a_p = a_c \frac{1}{2}\sqrt{2}$ and α = 60°. The relation between the two cells is described by the transformation matrix $\boldsymbol{P}_1$ (*cf.* Table 1.5.1.1 and Fig. 1.5.1.4):

$$(\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\boldsymbol{P}_1 = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}. \tag{1.5.2.18}$$

(ii) The transformation matrix $\boldsymbol{P}_2$ between the rhombohedral primitive cell and the triple hexagonal cell (obverse setting) of the reference description is read from Table 1.5.1.1 (*cf.* Fig. 1.5.1.6):

$$(\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c) = (\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)\boldsymbol{P}_2 = (\mathbf{a}_p, \mathbf{b}_p, \mathbf{c}_p)\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}. \tag{1.5.2.19}$$

Combining equations (1.5.2.18) and (1.5.2.19) gives the orientational relationship between the *F*-centred cubic cell and the rhombohedrally centred hexagonal cell $(\mathbf{a}'_c, \mathbf{b}'_c, \mathbf{c}'_c) = (\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c)\boldsymbol{P}$, where

$$\boldsymbol{P} = \boldsymbol{P}_1\boldsymbol{P}_2 = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & 0 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 1 \\ 0 & \frac{1}{2} & 1 \end{pmatrix}. \tag{1.5.2.20}$$

Formally, the lattice parameters of the reference unit cell can be extracted from the metric tensor $\boldsymbol{G}'_c$ obtained from the metric tensor $\boldsymbol{G}_c$ transformed by $\boldsymbol{P}$, *cf.* equation (1.5.2.4):

$$\begin{aligned} \boldsymbol{G}'_c &= \boldsymbol{P}^T\boldsymbol{G}_c\boldsymbol{P} \\ &= \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} \\ 1 & 1 & 1 \end{pmatrix}\begin{pmatrix} a_c^2 & 0 & 0 \\ 0 & a_c^2 & 0 \\ 0 & 0 & a_c^2 \end{pmatrix}\begin{pmatrix} -\frac{1}{2} & 0 & 1 \\ \frac{1}{2} & -\frac{1}{2} & 1 \\ 0 & \frac{1}{2} & 1 \end{pmatrix} \\ &= a_c^2\begin{pmatrix} \frac{1}{2} & -\frac{1}{4} & 0 \\ -\frac{1}{4} & \frac{1}{2} & 0 \\ 0 & 0 & 3 \end{pmatrix}, \end{aligned} \tag{1.5.2.21}$$

which gives $a'_c = a_c \frac{1}{2}\sqrt{2}$ = 4.249 Å and $c'_c = a_c\sqrt{3}$ = 10.408 Å. The comparison of these values with the experimentally deter-

mined lattice parameters of the low-symmetry phase [a_{hex} = 4.164 (2) Å, c_{hex} = 10.69 (4) Å (Chattopadhyay *et al.*, 1987)] determines the lattice deformation accompanying the displacive phase transition, which basically consists of expanding the cubic unit cell along the [111] direction. (In fact, the elongation along [111] is accompanied by a contraction in the *ab* plane that leads to an overall volume reduction of about 1.3%.)

Owing to the polar character of *R*3*m*, the symmetry conditions following from the group–subgroup relation $Fm\bar{3}m > R3m$ [*cf.* equation (1.5.2.11)] are not sufficient to determine the origin shift of the transformation between the high- and the low-symmetry space groups. The origin shift of $\boldsymbol{p} = (-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4})$ in this specific case is chosen in such a way that the relative displacements of Ge and Te are equal in size but in opposite direction along [111].

The inverse transformation matrix–column pair $(\boldsymbol{Q}, \boldsymbol{q}) = (\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{P}^{-1}, -\boldsymbol{P}^{-1}\boldsymbol{p})$ is necessary for the calculation of the atomic coordinates of the reference description X'_c. Given the matrix $\boldsymbol{P}$, its inverse $\boldsymbol{P}^{-1}$ can be calculated either directly (*i.e.* applying the algebraic procedure for inversion of a matrix) or using the inverse matrices $\boldsymbol{Q}_1 = \boldsymbol{P}_1^{-1}$ and $\boldsymbol{Q}_2 = \boldsymbol{P}_2^{-1}$ listed in Table 1.5.1.1:

$$\boldsymbol{Q} = \boldsymbol{P}^{-1} = (\boldsymbol{P}_1\boldsymbol{P}_2)^{-1} = \boldsymbol{P}_2^{-1}\boldsymbol{P}_1^{-1} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \bar{1} & 1 & 1 \\ 1 & \bar{1} & 1 \\ 1 & 1 & \bar{1} \end{pmatrix} = \begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}. \quad (1.5.2.22)$$

(Note the change in the order of multiplication of the matrices $\boldsymbol{P}_1^{-1}$ and $\boldsymbol{P}_2^{-1}$ in $\boldsymbol{Q}$.) The corresponding origin shift $\boldsymbol{q}$ is given by

$$\boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p} = -\begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} -\frac{1}{4} \\ -\frac{1}{4} \\ -\frac{1}{4} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}. \quad (1.5.2.23)$$

The atomic positions of the reference description become

$$\begin{pmatrix} x'_c \\ y'_c \\ z'_c \end{pmatrix} = \begin{pmatrix} -\frac{4}{3} & \frac{2}{3} & \frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} & \frac{4}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}.$$

The coordinates of the representative Ge atom occupying position 4*a* 0, 0, 0 in $Fm\bar{3}m$ are transformed to $0, 0, \frac{1}{4}$, while those of Te are transformed from 4*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ in $Fm\bar{3}m$ to $0, 0, \frac{3}{4}$. The comparison of these values with the experimentally determined atomic coordinates of Ge 0, 0, 0.2376 and Te 0, 0, 0.7624 reveals the corresponding atomic displacements associated with the displacive phase transition. The low-symmetry phase is a result of relative atomic displacements of the Ge and Te atoms along the polar (rhombohedral) [111] direction, giving rise to non-zero polarization along the same direction, *i.e.* the phase transition is a *paraelectric-to-ferroelectric* one.

1.5.3. Transformations between different space-group descriptions

By G. Chapuis, H. Wondratschek and M. I. Aroyo

1.5.3.1. Space groups with more than one description in this volume

In the description of the space-group symbols presented in Section 1.4.1, we have already seen that in the conventional, *unique axis b* description of monoclinic space groups, the unique symmetry direction is chosen as **b**; it is normal to **c** and **a**, which form the angle β. However, it is often the case that this standard direction is not the most appropriate choice and that another choice would be more convenient. An example of this would be when following a phase transition from an orthorhombic parent phase to a monoclinic phase. Here, it would often be preferable to keep the same orientation of the axes even if the resulting monoclinic setting is not standard.

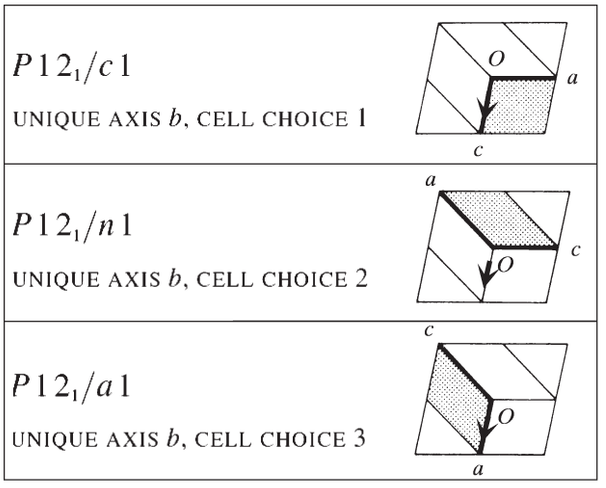


Figure 1.5.3.1
Three possible cell choices for the monoclinic space group $P2_1/c$ (14) with unique axis *b*. Note the corresponding changes in the full Hermann–Mauguin symbols. The glide vector is indicated by an arrow.

In some of the space groups, and especially in the monoclinic ones, the space-group tables of Chapter 2.3 provide a selection of possible alternative settings. For example, in space group $P2_1/c$, two possible orientations of the unit-cell axes are provided, namely with unique axis *b* and *c*. This is reflected in the corresponding full Hermann–Mauguin symbols by the explicit specification of the unique-axis position (dummy indices '1' indicate 'empty' symmetry directions), and by the corresponding change in the direction of the glide plane: $P12_1/c1$ or $P112_1/a$ (*cf.* Section 1.4.1 for a detailed treatment of Hermann–Mauguin symbols of space groups).

It is not just the unique monoclinic axis that can be varied: the choice of the other axes can vary as well. There are cases where the selection of the conventional setting leads to an inconvenient monoclinic angle that deviates greatly from 90°. If another cell choice minimizes the deviation from 90°, it is preferred. Fig. 1.5.3.1 illustrates three cell choices for the monoclinic axis *b* setting of $P2_1/c$.

In centrosymmetric space groups the origin of the unit cell is located at an inversion centre ('origin choice 2'). If, however, another point has higher site symmetry $\mathcal{S}$, a second diagram is displayed with the origin at a point with site symmetry $\mathcal{S}$ ('origin choice 1'). Fig. 1.5.3.2 illustrates the space group *Pban* with two possible origins. The origin of the first choice is located on a point with site symmetry 222, whereas the origin for the second choice is located on an inversion centre. Among the 230 space groups, this volume lists 24 centrosymmetric space groups with an additional alternative origin.

Finally, the seven rhombohedral space-group types (*i.e.* space groups with a rhombohedral lattice) also have alternative descriptions included in the space-group tables of this volume. The rhombohedral lattice is first presented with an *R*-centred

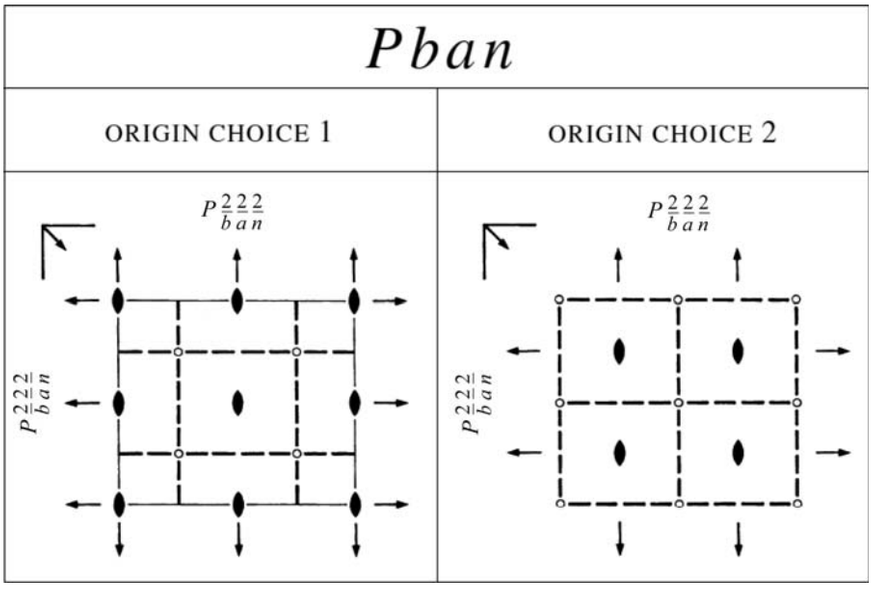


Figure 1.5.3.2
Two possible origin choices for the orthorhombic space group *Pban* (50). Origin choice 1 is on 222, whereas origin choice 2 is on $\bar{1}$.

hexagonal cell ($|\mathbf{a}_{\rm hex}| = |\mathbf{b}_{\rm hex}|$; $\mathbf{c}_{\rm hex} \perp \mathbf{a}_{\rm hex}, \mathbf{b}_{\rm hex}$; $\gamma = 120^\circ$) with a volume three times larger than that of the primitive rhombohedral cell. The second presentation is given with a primitive rhombohedral cell with $a_{\rm rh} = b_{\rm rh} = c_{\rm rh}$ and $\alpha_{\rm rh} = \beta_{\rm rh} = \gamma_{\rm rh}$. The relation between the two types of cell is illustrated in Fig. 1.5.3.3 for the space group *R*3*m* (160). In the hexagonal cell, the coordinates of the special position with site symmetry 3*m* are 0, 0, *z*, whereas in the rhombohedral cell the same special position has coordinates x, x, x. If we refer to the transformations of the primitive rhombohedral cell cited in Table 1.5.1.1, we observe two different centrings with three possible orientations R_1, R_2 and R_3 which are related by $\pm 120^\circ$ to each other. The two kinds of centrings, called *obverse* and *reverse*, are illustrated in Fig. 1.5.1.6. A rotation of 180° around the rhombohedral axis relates the obverse and reverse descriptions of the rhombohedral lattice. The obverse triple *R* cells have lattice points at $0, 0, 0$; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$, whereas the reverse *R* cells have lattice points at $0, 0, 0$; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$. The triple hexagonal cell R_1 of the obverse setting (*i.e.* $\mathbf{a}_{\rm hex} = \mathbf{a}_{\rm rh} - \mathbf{b}_{\rm rh}$, $\mathbf{b}_{\rm hex} = \mathbf{b}_{\rm rh} - \mathbf{c}_{\rm rh}$, $\mathbf{c}_{\rm hex} = \mathbf{a}_{\rm rh} + \mathbf{b}_{\rm rh} + \mathbf{b}_{\rm rh}$) has been used in the description of the rhombohedral space groups in this volume (*cf.* Table 1.5.1.1 and Fig. 1.5.3.3).

The hexagonal lattice can be referred to a centred rhombohedral cell, called the *D* cell (*cf.* Table 1.5.1.1). The centring points of this cell are $0, 0, 0$, $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$ and $\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$. However, the *D* cell is rarely used in crystallography.

1.5.3.2. Examples

1.5.3.2.1. Transformations between different settings of $P2_1/c$

In the space-group tables of this volume, the monoclinic space group $P2_1/c$ (14) is described in six different settings: for each of the 'unique axis *b*' and 'unique axis *c*' settings there are three descriptions specified by different cell choices (*cf.* Section 2.1.3.15). The different settings are identified by the appropriate full Hermann–Mauguin symbols. The basis transformations $(\boldsymbol{P}, \boldsymbol{p})$ between the different settings are completely specified by the linear part of the transformation, the 3×3 matrix $\boldsymbol{P}$ [*cf.* equation (1.5.1.4)], as all settings of $P2_1/c$ refer to the same origin, *i.e.* $\boldsymbol{p} = \boldsymbol{o}$. The transformation matrices $\boldsymbol{P}$ necessary for switching between the different descriptions of $P2_1/c$ can either be read off directly or constructed from the transformation-matrix data listed in Table 1.5.1.1.

(*A*) *Transformation from $P12_1/c1$ (unique axis b, cell choice 1) to $P112_1/a$ (unique axis c, cell choice 1)*. The change of the direction of the screw axis 2_1 indicates that the unique direction **b**

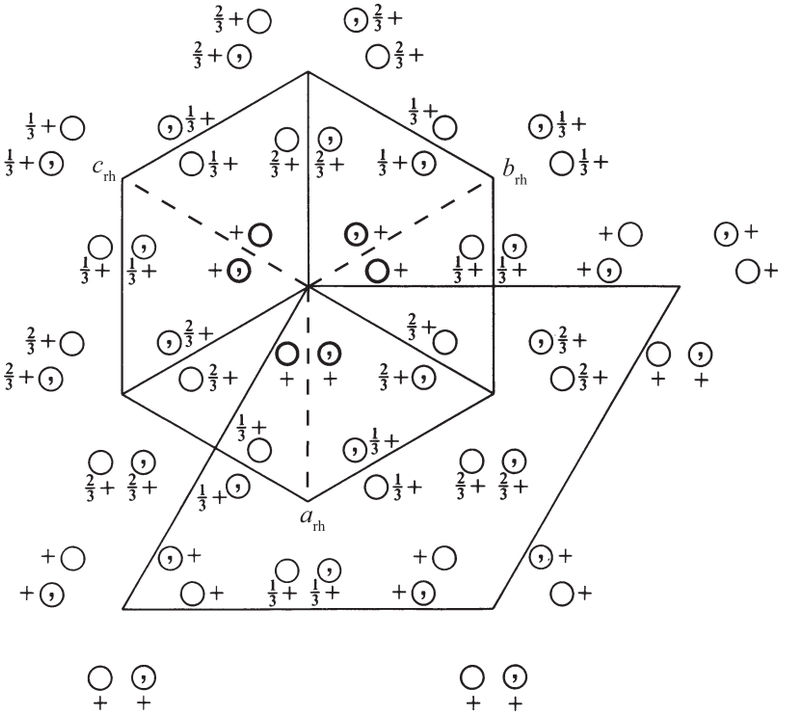


Figure 1.5.3.3
General-position diagram of the space group *R*3*m* (160) showing the relation between the hexagonal and rhombohedral axes in the obverse setting: $\mathbf{a}_{\rm rh} = \frac{1}{3}(2\mathbf{a}_{\rm hex} + \mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$, $\mathbf{b}_{\rm rh} = \frac{1}{3}(-\mathbf{a}_{\rm hex} + \mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$, $\mathbf{c}_{\rm rh} = \frac{1}{3}(-\mathbf{a}_{\rm hex} - 2\mathbf{b}_{\rm hex} + \mathbf{c}_{\rm hex})$.

Table 1.5.3.1
Transformation of reflection-condition data for $P12_1/c1$ to $P112_1/a$

	$P12_1/c1$ $h_bk_bl_b$	$P112_1/a$ $h_ck_cl_c$
General conditions	$h0l$: $l = 2n$ $0k0$: $k = 2n$ $00l$: $l = 2n$	$hk0$: $h = 2n$ $00l$: $l = 2n$ $h00$: $h = 2n$
Special conditions for the inversion centres	hkl: $k + l = 2n$	hkl: $h + l = 2n$

transforms to the unique direction **c**, while the glide vector along **c** transforms to a glide vector along **a**. These changes are reflected in the transformation matrix $\boldsymbol{P}$ between the basis $\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b$ of $P12_1/c1$ and $\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c$ of $P112_1/a$, which can be read directly from Table 1.5.1.1:

$$(\mathbf{a}_c, \mathbf{b}_c, \mathbf{c}_c) = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\boldsymbol{P} = (\mathbf{a}_b, \mathbf{b}_b, \mathbf{c}_b)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

(i) *Transformation of point coordinates*. From $\boldsymbol{x}' = \boldsymbol{P}^{-1}\boldsymbol{x}$, *cf.* equation (1.5.1.5), it follows that

$$\begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} x_b \\ y_b \\ z_b \end{pmatrix} = \begin{pmatrix} z_b \\ x_b \\ y_b \end{pmatrix}.$$

For example, the representative coordinate triplets of the special Wyckoff position $2d\ \bar{1}$ of $P12_1/c1$ transform exactly to the representative coordinate triplets of the special Wyckoff position $2d\ \bar{1}$ of $P112_1/a$: $\begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}$ and $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ transform to $\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$.

(ii) *Transformation of the indices in the 'Reflection conditions' block*. Under a coordinate transformation specified by a matrix $\boldsymbol{P}$, the indices of the reflection conditions (Miller indices) transform according to $(h'k'l') = (hkl)\boldsymbol{P}$, *cf.* equation (1.5.2.2). The transformation under

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

of the set of general or special reflection conditions $h_bk_bl_b$ for $P12_1/c1$ should result in the set of general or special reflection conditions $h_ck_cl_c$ of $P112_1/a$:

$$(h_ck_cl_c) = (h_bk_bl_b)\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (l_bh_bk_b),$$

i.e. $h_c = l_b, k_c = h_b, l_c = k_b$ (see Table 1.5.3.1).

(iii) *Transformation of the matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$ *of the symmetry operations*. The matrices of the representatives of the symmetry operations of $P12_1/c1$ can be constructed from the coordinate triplets listed in the general-position block of the group:

(1) x, y, z (2) $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (3) $\bar{x}, \bar{y}, \bar{z}$ (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$

Their transformation is more conveniently performed using the augmented-matrix formalism. According to equation (1.5.2.17), the matrices $\mathbb{W}_c$ of the symmetry operations of $P112_1/a$ are related to the matrices $\mathbb{W}_b$ of $P12_1/c1$ by the equation $\mathbb{W}_c = \mathbb{Q}\mathbb{W}_b\mathbb{P}$, where

$$\mathbb{P} = \left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \quad \text{and} \quad \mathbb{Q} = \left(\begin{array}{ccc|c} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

The unit matrix representing the identity operation (1) is invariant under any basis transformation, *i.e.* x, y, z transforms to x, y, z. Similarly, the matrix of inversion $\bar{1}$ (3) (the linear part of which is a multiple of the unit matrix) is also invariant under any basis transformation, *i.e.* $\bar{x}, \bar{y}, \bar{z}$ transforms to $\bar{x}, \bar{y}, \bar{z}$. The symmetry operation (2) $\bar{x},\ y + \frac{1}{2},\ \bar{z} + \frac{1}{2}$, represented by the matrix

$$\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$

transforms to

$$\left(\begin{array}{ccc|c} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)\left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right)\left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right)$$
$$= \left(\begin{array}{ccc|c} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

which corresponds to $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$.

Finally, the symmetry operation (4) $x, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ represented by the matrix

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \text{ transforms to } \left(\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

corresponding to the coordinate triplet $x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ [the matrices of (4) and its transformed are those of (2) and its transformed, multiplied by $\bar{1}$].

The coordinate triplets of the transformed symmetry operations correspond to the entries of the general-position block of $P112_1/a$ (*cf.* the space-group tables of $P2_1/c$ in Chapter 2.3).

(*B*) *Transformation from* $P112_1/b$ *(unique axis c, cell choice 3) to* $P12_1/c1$ *(unique axis b, cell choice 1)*: $(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}$. A transformation matrix from $P112_1/b$ directly to $P12_1/c1$ is not found in Table 1.5.1.1, but it can be constructed in two steps from transformation matrices that are listed there. For example:

Step 1. Unique axis *c* fixed: transformation from 'cell choice 3' to 'cell choice 1':

$$(\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1}) = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}_1 = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (1.5.3.1)$$

Step 2. Cell choice 1 invariant: transformation from unique axis c to unique axis b:

$$(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) = (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\boldsymbol{P}_2 = (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \quad (1.5.3.2)$$

The transformation matrix $\boldsymbol{P}$ for the change from $P112_1/b$ to $P12_1/c1$ is obtained by starting from equation (1.5.3.2) and replacing the expression for $\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1}$ with that from equation (1.5.3.1):

$$\begin{aligned}(\mathbf{a}_{b,1}, \mathbf{b}_{b,1}, \mathbf{c}_{b,1}) &= (\mathbf{a}_{c,1}, \mathbf{b}_{c,1}, \mathbf{c}_{c,1})\boldsymbol{P}_2 = (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\boldsymbol{P}_1\boldsymbol{P}_2 \\ &= (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\ &= (\mathbf{a}_{c,3}, \mathbf{b}_{c,3}, \mathbf{c}_{c,3})\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.\end{aligned}$$

The inverse matrix $\boldsymbol{Q} = \boldsymbol{P}^{-1}$ can be obtained either by inversion or by the product of the factors $\boldsymbol{Q}_1 = \boldsymbol{P}_1^{-1}$ and $\boldsymbol{Q}_2 = \boldsymbol{P}_2^{-1}$ but in reverse order:

$$\boldsymbol{Q} = (\boldsymbol{P}_1\boldsymbol{P}_2)^{-1} = \boldsymbol{P}_2^{-1}\boldsymbol{P}_1^{-1} = \boldsymbol{Q}_2\boldsymbol{Q}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ \bar{1} & 1 & 0 \end{pmatrix}.$$

The transformation matrix $\boldsymbol{P}$ determined above and its inverse $\boldsymbol{Q}$ permit the transformation of crystallographic data for the change from $P112_1/b$ to $P12_1/c1$.

1.5.3.2.2. Transformation between the two origin-choice settings of $I4_1/amd$

The zircon example of Section 1.5.1.1 illustrates how the atomic coordinates change under an origin-choice transformation. Here, the case of the two origin-choice descriptions of the same space group $I4_1/amd$ (141) will be used to demonstrate how the rest of the crystallographic quantities are affected by an origin shift.

The two descriptions of $I4_1/amd$ in the space-group tables of this volume are distinguished by the origin choices of the reference coordinate systems: the origin statement of the origin choice 1 setting indicates that its origin O_1 is taken at a point of $\bar{4}m2$ symmetry, which is located at $0, \frac{1}{4}, -\frac{1}{8}$ with respect to the origin O_2 of origin choice 2, taken at a centre $(2/m)$. Conversely, the origin O_2 is taken at a centre $(2/m)$ at $0, -\frac{1}{4}, \frac{1}{8}$ from the origin O_1. These origin descriptions in fact specify explicitly the origin-shift vector $\boldsymbol{p}$ necessary for the transformation between the two settings. For example, the shift vector listed for origin choice 2 expresses the origin O_2 with respect to O_1, *i.e.* the corresponding transformation matrix

$$(\boldsymbol{P}, \boldsymbol{p}) = (\boldsymbol{I}, \boldsymbol{p}) = \left(\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ -\frac{1}{4} \\ \frac{1}{8} \end{pmatrix}\right)$$

transforms the crystallographic data from the origin choice 1 setting to the origin choice 2 setting.

(i) *Transformation of point coordinates.* In accordance with the discussion of Section 1.5.1.1 [*cf.* equation (1.5.1.2)], the transformation of point coordinates $\boldsymbol{x}_1 = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$ of the origin choice 1 setting of $I4_1/amd$ to $\boldsymbol{x}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$ of the origin choice 2 setting is given by

$$\boldsymbol{x}_2 = \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix} = (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x}_1 = (\boldsymbol{I}, -\boldsymbol{p})\boldsymbol{x}_1 = \begin{pmatrix} x_1 \\ y_1 + \frac{1}{4} \\ z_1 - \frac{1}{8} \end{pmatrix}. \quad (1.5.3.3)$$

(ii) *Metric tensors and the data for the reflection conditions*. The metric tensors and the data for the reflection conditions are not affected by an origin shift as $\boldsymbol{P} = \boldsymbol{I}$, *cf.* equations (1.5.2.4) and (1.5.2.2).

(iii) *Transformation of the matrix–column pairs* $(\boldsymbol{W}, \boldsymbol{w})$ *of the symmetry operations*. The origin-shift transformation $(\boldsymbol{I}, \boldsymbol{p})$ relates the matrix–column pairs $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ of the symmetry operations of the origin choice 1 setting of $I4_1/amd$ to $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ of the origin choice 2 setting [*cf.* equation (1.5.2.11)]:

$$(\boldsymbol{W}_2, \boldsymbol{w}_2) = (\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}_1, \boldsymbol{w}_1)(\boldsymbol{I}, \boldsymbol{p}) = (\boldsymbol{W}_1, \boldsymbol{w}_1 + [\boldsymbol{W}_1 - \boldsymbol{I}]\boldsymbol{p}). \quad (1.5.3.4)$$

The rotation part of the symmetry operation is not affected by the origin shift, but the translation part is affected, *i.e.* $\boldsymbol{W}_2 = \boldsymbol{W}_1$ and $\boldsymbol{w}_2 = \boldsymbol{w}_1 + [\boldsymbol{W}_1 - \boldsymbol{I}]\boldsymbol{p}$. For example, the translation and unit element generators of $I4_1/amd$ are not changed under the origin-shift transformation, as $\boldsymbol{W}_1 = \boldsymbol{I}$. The first non-translation generator given by the coordinate triplet $\bar{y}, x + \frac{1}{2}, z + \frac{1}{4}$ and represented by the matrix

$$\left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}\right) \text{ transforms to } \left(\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} \frac{1}{4} \\ \frac{3}{4} \\ \frac{1}{4} \end{pmatrix}\right),$$

which corresponds to the coordinate triplet $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$.

The second non-translation generator $\bar{x}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$, represented by the matrix

$$\left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{pmatrix}\right) \text{ transforms to } \left(\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\right),$$

which under the normalization $0 \leq w_i < 1$ is written as the coordinate triplet $\bar{x}, \bar{y}, \bar{z}$. The coordinate triplets of the transformed symmetry operations are the entries of the corresponding generators of the origin choice 2 setting of $I4_1/amd$ (*cf.* the space-group tables of $I4_1/amd$ in Chapter 2.3).

1.5.4. Synoptic tables of plane and space groups[2]

By B. Souvignier, G. Chapuis and H. Wondratschek

It is already clear from Section 1.5.3.1 that the Hermann–Mauguin symbols of a space group depend on the choice of the basis vectors. The purpose of this section is to give an overview of a large selection of possible alternative settings of space groups and their Hermann–Mauguin symbols covering most practical cases. In particular, the synoptic tables include two main types of information:

(i) Space-group symbols for various settings and choices of the basis. The axis transformations involve permutations of axes conserving the shape of the cell and also transformations leading to different cell shapes and multiple cells.

(ii) *Extended* Hermann–Mauguin space-group symbols in addition to the short and full symbols. The three types of symbols, short, full and extended, provide different levels of information about the symmetry elements and the related symmetry operations of the space group (*cf.* Section 1.2.3 for definitions and discussion of the concepts of symmetry element, geometric element, element set and defining symmetry operation). The short and full Hermann–Mauguin symbols only display information about a chosen set of generators for a space group from which all the elements of a space group can in principle be deduced (*cf.* Section 1.4.1.4 for a detailed treatment of short and full Hermann–Mauguin symbols). The multiplicity of the general position in each space group gives the number of symmetry operations *modulo* the lattice translations. As already discussed in Section 1.4.2.4, the combinations of this representative set of symmetry operations with lattice translations give rise to *additional symmetry operations* and *additional symmetry elements*, displayed in the symmetry-element diagrams. The additional symmetry operations are also reflected in the so-called *extended Hermann–Mauguin symbols*, which were introduced in *International Tables for X-ray Crystallography* Volume I (1952). They were systematically developed and tabulated by Bertaut for the first edition of Volume A of *International Tables for Crystallography* (*IT* A), published in 1983. The background for the correct construction and interpretation of the extended Hermann–Mauguin symbols is presented in the following section.

1.5.4.1. Additional symmetry operations and symmetry elements

In order to interpret (or even determine) the extended symbol for a space group, one has to recall that all operations that belong to the same coset with respect to the translation subgroup have the same linear part, but that not all symmetry operations within a coset are operations of the same type. Furthermore, symmetry operations in one coset can belong to element sets of different symmetry elements.

1.5.4.1.1. Determining the type of a symmetry operation

In this section, a procedure for determining the types of symmetry operations and the corresponding symmetry elements is explained. It is a development of the method of geometrical interpretation discussed in Section 1.2.2.4. The procedure is based on the origin-shift transformations discussed in Sections 1.5.1 and 1.5.2, and provides an efficient way of analysing the additional symmetry operations and symmetry elements. The key to the procedure is the decomposition of the translation part $\boldsymbol{w}$ of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ into an *intrinsic translation part* $\boldsymbol{w}_g$, which is fixed by the linear part $\boldsymbol{W}$ of W and thus parallel to the geometric element of W, and a *location part* $\boldsymbol{w}_l$, which is perpendicular to the intrinsic translation part. Note that the space fixed by $\boldsymbol{W}$ and the space perpendicular to this fixed space are complementary, *i.e.* their dimensions add up to 3, therefore this decomposition is always possible.

As described in Section 1.2.2.4, the determination of the intrinsic translation part of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ with linear part $\boldsymbol{W}$ of order k is based on the fact that the kth power of W must be a pure translation, *i.e.* $W^k = (\boldsymbol{I}, \boldsymbol{t})$ for some lattice translation t. The *intrinsic translation part* of W is then defined as $\boldsymbol{w}_g = (1/k)\boldsymbol{t}$.

The difference $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{w}_g$ is perpendicular to $\boldsymbol{w}_g$ and it is called the *location part* of $\boldsymbol{w}$. This terminology is justified by the following observation: As explained in detail in Sections 1.5.1.3 and 1.5.2.3, under an origin shift by $\boldsymbol{p}$, a column $\boldsymbol{x}$ of point coordinates is transformed to

$$\boldsymbol{x}' = (\boldsymbol{I}, -\boldsymbol{p})\boldsymbol{x} = (\boldsymbol{I}, \boldsymbol{p})^{-1}\boldsymbol{x},$$

making in particular $\boldsymbol{p}$ the new origin, and a matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$ is transformed to

$$(\boldsymbol{W}', \boldsymbol{w}') = (\boldsymbol{I}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}, \boldsymbol{p}).$$

Applied to the symmetry operation $(\boldsymbol{W}, \boldsymbol{w}_l)$, known as the *reduced symmetry operation* in which the full translation part is replaced by the location part (thereby neglecting the intrinsic translation part), an origin shift by $\boldsymbol{p}$ results in

$$\begin{aligned}(\boldsymbol{I}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w}_l)(\boldsymbol{I}, \boldsymbol{p}) &= (\boldsymbol{I}, -\boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w}_l)(\boldsymbol{I}, \boldsymbol{p}) \\ &= (\boldsymbol{W}, \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p} + \boldsymbol{w}_l) \\ &= (\boldsymbol{W}, (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p} + \boldsymbol{w}_l).\end{aligned}$$

This means that if it is possible to find an origin shift $\boldsymbol{p}$ such that $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}_l$, then with respect to the new origin the reduced symmetry operation $(\boldsymbol{W}, \boldsymbol{w}_l)$ is transformed to $(\boldsymbol{W}, \boldsymbol{o})$. But since the subspace perpendicular to the fixed space of $\boldsymbol{W}$ clearly does not contain any vector fixed by $\boldsymbol{W}$, the restriction of $\boldsymbol{I} - \boldsymbol{W}$ to this subspace is an invertible linear transformation, and therefore for every location part $\boldsymbol{w}_l$ there is indeed a suitable $\boldsymbol{p}$ perpendicular to the fixed space of $\boldsymbol{W}$ such that $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}_l$.

The fact that an origin shift by $\boldsymbol{p}$ transforms the translation part of the reduced symmetry operation $(\boldsymbol{W}, \boldsymbol{w}_l)$ to $\boldsymbol{o}$ is equivalent to $\boldsymbol{p}$ being a fixed point of $(\boldsymbol{W}, \boldsymbol{w}_l)$, which can also be seen directly because

$$(\boldsymbol{W}, \boldsymbol{w}_l)\boldsymbol{p} = \boldsymbol{W}\boldsymbol{p} + \boldsymbol{w}_l = \boldsymbol{W}\boldsymbol{p} + (\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{p}.$$

Note that for one fixed point $\boldsymbol{p}$ of the reduced symmetry operation $(\boldsymbol{W}, \boldsymbol{w}_l)$, the full *set of fixed points*, as defined in Section 1.2.4, is obtained by adding $\boldsymbol{p}$ to the fixed vectors of $\boldsymbol{W}$, because for an arbitrary fixed point $\boldsymbol{p}_F$ of $(\boldsymbol{W}, \boldsymbol{w}_l)$ one has $\boldsymbol{W}\boldsymbol{p}_F + \boldsymbol{w}_l = \boldsymbol{p}_F$ and since also $\boldsymbol{W}\boldsymbol{p} + \boldsymbol{w}_l = \boldsymbol{p}$ one finds $\boldsymbol{W}(\boldsymbol{p}_F - \boldsymbol{p}) = \boldsymbol{p}_F - \boldsymbol{p}$, *i.e.* the difference between two fixed points is a vector that is fixed by $\boldsymbol{W}$. In other words, the geometric element of $(\boldsymbol{W}, \boldsymbol{w}_l)$ is the space fixed by $\boldsymbol{W}$, translated such that it runs through $\boldsymbol{p}$.

Finally, in order to determine the symmetry element of the symmetry operation correctly, it may be necessary to reduce the intrinsic translation part $\boldsymbol{w}_g$ by a lattice translation in the fixed space of $\boldsymbol{W}$.

[2] With Tables 1.5.4.1, 1.5.4.2, 1.5.4.3 and 1.5.4.4 by E. F. Bertaut.

Summarizing, the types of symmetry operations $W = (\boldsymbol{W}, \boldsymbol{w})$ and their symmetry elements can be identified as follows:

(i) Decompose the translation part $\boldsymbol{w}$ as $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$, where $\boldsymbol{w}_g$ and $\boldsymbol{w}_l$ are mutually perpendicular and the intrinsic translation part $\boldsymbol{w}_g$ is fixed by the linear part $\boldsymbol{W}$ of W.

(ii) Determine a shift of origin $\boldsymbol{p}$ such that $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}_l$, *i.e.* such that $\boldsymbol{p}$ is a fixed point of the reduced operation $(\boldsymbol{W}, \boldsymbol{w}_l)$.

(iii) For the correct determination of the defining operation of the symmetry element it may be necessary to reduce the intrinsic translation part $\boldsymbol{w}_g$ by a lattice translation in the fixed space of $\boldsymbol{W}$, thus yielding a coplanar or coaxial equivalent symmetry operation.

This analysis allows one to read off the types of the symmetry operations and of the corresponding symmetry elements that occur for the coset $\mathcal{T}W$ of W. The following two sections provide examples illustrating that in some cases the coset does not contain symmetry operations belonging to symmetry elements of different type, while in others it does.

1.5.4.1.2. Cosets without additional types of symmetry elements

In cases where the linear part $\boldsymbol{W}$ of a symmetry operation W fixes only the origin, all elements in the coset are of the same type. This is due to the fact that the translation part $\boldsymbol{w}$ is decomposed as $\boldsymbol{w}_g = \boldsymbol{o}$ and $\boldsymbol{w}_l = \boldsymbol{w}$. Since $\boldsymbol{W}$ fixes only the origin, $\boldsymbol{I} - \boldsymbol{W}$ is invertible and a fixed point $\boldsymbol{p}$ of the reduced operation $(\boldsymbol{W}, \boldsymbol{w}_l) = (\boldsymbol{W}, \boldsymbol{w})$ can be found, as $\boldsymbol{p} = (\boldsymbol{I} - \boldsymbol{W})^{-1}\boldsymbol{w}$. This situation occurs when W is an inversion or a three-, four- or sixfold rotoinversion. The element set of the symmetry element of an inversion consists only of this inversion; the element set of a rotoinversion consists of the rotoinversion W and its inverse W^{-1} (the latter belonging to a different coset). Therefore, in these cases each symmetry operation in the coset of W belongs to the element set of a different symmetry element (of the same type, namely an inversion centre or a rotoinversion axis).

Note that the above argument does not apply to twofold rotoinversions, since these are in fact reflections which fix a plane perpendicular to the rotoinversion axis and not only a single point. The following two examples illustrate that translations from a primitive lattice do not give rise to symmetry elements of different type in the cases of either a reflection or glide reflection with normal vector along one of the coordinate axes, or of a rotation or screw rotation with rotation axis along one of the coordinate axes.

Example 1

Let $W = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ be an n glide with normal vector along the c axis. For the composition of W with an integral translation $t(u_1, u_2, u_3)$ one obtains a symmetry operation W' with translation part $\boldsymbol{w}' = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ u_3 \end{pmatrix}$. The decomposition of $\boldsymbol{w}'$ into the intrinsic translation part and the location part gives $\boldsymbol{w}'_g = \begin{pmatrix} u_1 + \frac{1}{2} \\ u_2 + \frac{1}{2} \\ 0 \end{pmatrix}$ and $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$. This shows that the intrinsic translation part is only changed by the lattice vector $\begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$ and hence W' is a coplanar equivalent of the symmetry operation $W'' = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + u_3$, which is an n glide with glide plane normal to the c axis and located at $z = u_3/2$. One concludes that W and W' belong to symmetry elements of the same type. The same conclusion would in fact remain true in the case of a C-centred lattice, since the composition of W with the centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ would simply result in the intrinsic translation part being changed by the centring translation.

Example 2

As an example of a rotation, let $W = \bar{y}, x, z$ be a fourfold rotation $4^+\ 0, 0, z$ around the c axis. Composing W with the translation $t(u_1, u_2, u_3)$ results in the symmetry operation $W' = \bar{y} + u_1, x + u_2, z + u_3$ with intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} 0 \\ 0 \\ u_3 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$. Since we assume a primitive lattice, u_3 is an integer, hence W' is a coaxial equivalent of the symmetry operation $W'' = \bar{y} + u_1, x + u_2, z$, which has intrinsic translation part $\boldsymbol{o}$. To locate the geometric element of W', one notes that for

$$\boldsymbol{W} = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

one has

$$(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l \text{ for } \boldsymbol{p} = \begin{pmatrix} (u_1 - u_2)/2 \\ (u_1 + u_2)/2 \\ 0 \end{pmatrix}.$$

The symmetry operation W' therefore belongs to the symmetry element of a fourfold rotation with the line $(u_1 - u_2)/2, (u_1 + u_2)/2, z$ as geometric element. This analysis shows that all symmetry operations in the coset $\mathcal{T}W$ belong to the same type of symmetry element, since for each of these symmetry operations a coaxial equivalent can be found that has zero screw component.

1.5.4.1.3. Examples with additional types of symmetry elements

The examples given in the previous section illustrate that in the case of a translation vector perpendicular to the symmetry axis or symmetry plane of a symmetry operation, the intrinsic translation vector remains unchanged and only the location of the geometric element is altered. In particular, composition with such a translation vector results in symmetry operations and symmetry elements of the same type. On the other hand, composition with translations parallel to the symmetry axis or symmetry plane give rise to coaxial or coplanar equivalents, which also belong to the same symmetry element. Combining these two observations shows that for integral translations, only translations along a direction inclined to the symmetry axis or symmetry plane can give rise to additional symmetry elements. For these cases, the additional symmetry operations and their locations are summarized in Table 1.5.4.1.

In space groups with a centred lattice, the translation subgroup contains also translations with non-integral components, and these often give rise to symmetry operations and symmetry elements of different types in the same coset. An overview of additional symmetry operations and their locations that occur due to centring vectors is given in Table 1.5.4.2. In rhombohedral space groups all additional types of symmetry elements occur already as a result of combinations with integral lattice translations (*cf.* Table 1.5.4.1). For this reason, the rhombohedral centring R case is not included in Table 1.5.4.2.

In Section 1.4.2.4 the occurrence of glide reflections in a space group of type $P4mm$ (due to integral translations inclined to a

Table 1.5.4.1
Additional symmetry operations and their locations if the translation vector **t** is inclined to the symmetry axis or symmetry plane

The table is restricted to integral translations and thus is valid for primitive lattices and for integral translations in centred lattices (for centring translations see Table 1.5.4.2).

Symmetry operation at the origin			Additional symmetry operation			Representative plane and space groups (numbers)
Symbol	Location	Translation vector **t**	Symbol	Screw or glide component	Location	
Tetragonal, rhombohedral and cubic coordinate systems						
2	$x, x, 0$	1, 0, 0 0, 1, 0	2_1	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, 0$	*P*422 (89) *R*32 (155) *P*432 (207)
m	x, x, z	1, 0, 0 0, 1, 0	*g*	$\frac{1}{2}, \frac{1}{2}, 0$ $\frac{1}{2}, \frac{1}{2}, 0$	$x, x+\frac{1}{2}, z$	*p*4*mm* (11) *P*4*mm* (99) *R*3*m* (160) $P\bar{4}3m$ (215)
c	x, x, z	1, 0, 0 0, 1, 0	*n*	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$x, x+\frac{1}{2}, z$	$P\bar{4}2c$ (112) *R*3*c* (161) $P\bar{4}3n$ (218)
Hexagonal coordinate system						
2	$x, 0, 0$	1, 1, 0 0, 1, 0	2_1	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, 0$	*P*321 (150) *R*32 (155)
2	$x, 2x, 0$	0, 1, 0 1, 1, 0	2_1	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, 0$	*P*312 (149) *P*622 (177)
m	$x, 2x, z$	0, 1, 0 1, 1, 0	*b*	$\frac{1}{2}, 1, 0$	$x, 2x+\frac{1}{2}, z$	*P*3*m*1 (156) *p*3*m*1 (14) *R*3*m* (160)
c	$x, 2x, z$	0, 1, 0 1, 1, 0	*n*	$\frac{1}{2}, 1, \frac{1}{2}$	$x, 2x+\frac{1}{2}, z$	*P*3*c*1 (158) $P\bar{6}c2$ (188) *R*3*c* (161)
m	$x, 0, z$	1, 1, 0 0, 1, 0	*a*	$\frac{1}{2}, 0, 0$ $-\frac{1}{2}, 0, 0$	$x, \frac{1}{2}, z$	*P*31*m* (157) *p*31*m* (15)
c	$x, 0, z$	1, 1, 0 0, 1, 0	*n*	$\frac{1}{2}, 0, \frac{1}{2}$ $-\frac{1}{2}, 0, \frac{1}{2}$	$x, \frac{1}{2}, z$	*P*31*c* (159) $P\bar{6}2c$ (190)
Rhombohedral and cubic coordinate systems						
3	x, x, x	1, 0, 0 0, 1, 0 0, 0, 1	3_1	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	$x, x+\frac{2}{3}, x+\frac{1}{3}$	*R*3 (146) *P*23 (195)
3	x, x, x	2, 0, 0 0, 2, 0 0, 0, 2	3_2	$\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$	$x, x+\frac{1}{3}, x+\frac{2}{3}$	

symmetry plane) and of type *Fmm*2 (due to centring translations) is discussed. We now provide some further examples illustrating the contents of Tables 1.5.4.1 and 1.5.4.2.

Example 3

Let $W = z, x, y$ be a threefold rotation 3^+ x, x, x along the [111] direction in a cubic (or rhombohedral) space group. Then the coset $\mathcal{T}W$ also contains the symmetry operation $W' = z+1, x, y$. With

$$\boldsymbol{W} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

one sees that $(W')^3 = t(1,1,1)$ and hence the intrinsic translation part is

$$\boldsymbol{w}'_g = \tfrac{1}{3}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix}.$$

It follows that the location part is $\boldsymbol{w}'_l = \begin{pmatrix} \frac{2}{3} \\ -\frac{1}{3} \\ -\frac{1}{3} \end{pmatrix}$ and one finds that $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} \frac{2}{3} \\ \frac{1}{3} \\ 0 \end{pmatrix}$. Thus, the symmetry operation $W' = z+1, x, y$ is of a different type to W: it is a threefold screw rotation $3^+(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ $x+\frac{2}{3}, x+\frac{1}{3}, x$ with the line $x+\frac{2}{3}, x+\frac{1}{3}, x$ as geometric element.

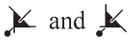
On the other hand, for an integer $u \neq 0$, the symmetry operation $W'' = z+u, x+u, y+u$ itself is a screw rotation, but it belongs to a symmetry element of rotation type, since it is a coaxial equivalent of the threefold rotation W. The crucial difference between the symmetry operations $W' = z+1, x, y$ and $W'' = z+u, x+u, y+u$ is that in the latter case the intrinsic translation part $\begin{pmatrix} u \\ u \\ u \end{pmatrix}$ is a lattice vector, whereas for $W' = z+1, x, y$ it is not.

Table 1.5.4.2
Additional symmetry operations due to a centring vector **t** and their locations

Symmetry operation at the origin		Additional symmetry operations									Representative space groups (numbers)
		$C, t(\frac{1}{2}, \frac{1}{2}, 0)$		$A, t(0, \frac{1}{2}, \frac{1}{2})$		$B, t(\frac{1}{2}, 0, \frac{1}{2})$		$I, t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		F	
Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	Location	Symbol	
m	$0, y, z$	b	$\frac{1}{4}, y, z$	n	$0, y, z$	c	$\frac{1}{4}, y, z$	n	$\frac{1}{4}, y, z$	b, n, c	*Cmmm*, *Ammm*, *Bmmm* (65)
c		n		b		m		b			*Immm* (71), *Fmmm* (69)
b		m		c		n		c			*Cccm*, *Amaa*, *Bbmb* (66), *Ibca* (73)
$d(0, \frac{1}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{1}{4})$		$d(0, \frac{3}{4}, \frac{3}{4})$		$d(0, \frac{1}{4}, \frac{3}{4})$				d, d, d	*Fddd* (70)
m	$x, 0, z$	a	$x, \frac{1}{4}, z$	c	$x, \frac{1}{4}, z$	n	$x, 0, z$	n	$x, \frac{1}{4}, z$	a, c, n	As above
a		m		n		c		c			
c		n		m		a		a			
$d(\frac{1}{4}, 0, \frac{1}{4})$		$d(\frac{3}{4}, 0, \frac{1}{4})$		$d(\frac{1}{4}, 0, \frac{3}{4})$		$d(\frac{3}{4}, 0, \frac{3}{4})$				d, d, d	
m	$x, y, 0$	n	$x, y, 0$	b	$x, y, \frac{1}{4}$	a	$x, y, \frac{1}{4}$	n	$x, y, \frac{1}{4}$	n, b, a	As above
b		a		m		n		a			
a		b		n		m		b			
$d(\frac{1}{4}, \frac{1}{4}, 0)$		$d(\frac{3}{4}, \frac{3}{4}, 0)$		$d(\frac{1}{4}, \frac{3}{4}, 0)$		$d(\frac{3}{4}, \frac{1}{4}, 0)$				d, d, d	
m	x, x, z	$g(\frac{1}{2}, \frac{1}{2}, 0)$	x, x, z	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x+\frac{1}{4}, z$	$g(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$	$x, x-\frac{1}{4}, z$	$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	x, x, z	g, g, g	*I*4*mm* (107), *F*$\bar{4}$3*m* (216)
c		$n(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{4}, \frac{1}{4}, 0)$		$g(\frac{1}{2}, \frac{1}{2}, 0)$		n, g, g	*F*$\bar{4}$3*c* (219)
$d(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$								$d(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$			*I*$\bar{4}$3*d* (220)
2	$x, 0, 0$	2_1	$x, \frac{1}{4}, 0$	2	$x, \frac{1}{4}, \frac{1}{4}$	2_1	$x, 0, \frac{1}{4}$	2_1	$x, \frac{1}{4}, \frac{1}{4}$	$2_1, 2, 2_1$	*C*222, *A*222, *B*222 (21)
2	$0, y, 0$	2_1	$\frac{1}{4}, y, 0$	2_1	$0, y, \frac{1}{4}$	2	$\frac{1}{4}, y, \frac{1}{4}$	2_1	$\frac{1}{4}, y, \frac{1}{4}$	$2_1, 2_1, 2$	*I*222 (23)
2	$0, 0, z$	2	$\frac{1}{4}, \frac{1}{4}, z$	2_1	$0, \frac{1}{4}, z$	2_1	$\frac{1}{4}, 0, z$	2_1	$\frac{1}{4}, \frac{1}{4}, z$	$2, 2_1, 2_1$	*F*222 (22)
2	$x, \bar{x}, 0$	2	$x, \bar{x}+\frac{1}{2}, 0$	$2_1(-\frac{1}{4}, \frac{1}{4}, 0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	$2_1(\frac{1}{4}, -\frac{1}{4}, 0)$	$x, \bar{x}+\frac{1}{4}, \frac{1}{4}$	2	$x, \bar{x}, \frac{1}{4}$	$2, 2_1, 2_1$	*C*422 (*P*422) (89), *I*422 (97)
4	$0, 0, z$	4	$0, \frac{1}{2}, z$	4_2	$-\frac{1}{4}, \frac{1}{4}, z$	4_2	$\frac{1}{4}, \frac{1}{4}, z$	4_2	$0, \frac{1}{2}, z$	$4, 4_2, 4_2$	*F*432 (209)
4_1	$0, 0, z$	4_1	$0, \frac{1}{2}, z$	4_3	$-\frac{1}{4}, \frac{1}{4}, z$	4_3	$\frac{1}{4}, \frac{1}{4}, z$	4_3	$0, \frac{1}{2}, z$	$4_1, 4_3, 4_3$	*F*4$_1$32 (210)
$\bar{1}$	$0, 0, 0$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, 0$	$\bar{1}$	$0, \frac{1}{4}, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, 0, \frac{1}{4}$	$\bar{1}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\bar{1}, \bar{1}, \bar{1}$	*Immm* (71), *Fmmm* (69)

This example illustrates in particular the occurrence of symmetry elements of screw or glide type even in the case of symmorphic space groups where all coset representatives $W = (\boldsymbol{W}, \boldsymbol{w})$ with respect to the translation subgroup can be chosen with $\boldsymbol{w} = \boldsymbol{o}$.

Note that, mainly for historical reasons, the screw rotations resulting from the threefold rotation along the [111] direction are not included in the extended Hermann–Mauguin symbol of cubic space groups, *cf.* Table 1.5.4.4. However, these screw rotations are represented in the cubic symmetry-element diagrams by the symbols



(*cf.* Table 2.1.2.7), as can be observed in the symmetry-element diagram for a group of type *P*23 (195) in Fig. 1.5.4.1.

Example 4

A twofold rotation $W = y, x, \bar{z}$ with the line $x, x, 0$ as geometric element has linear part

$$\boldsymbol{W} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}.$$

The composition W' of W with the translation $t(0, 1, 0)$ has intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$. Since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$, the symmetry operation $W' = y, x+\frac{1}{2}, \bar{z}$ is a screw rotation 2 $(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x+\frac{1}{2}, 0$ with the line $x, x+\frac{1}{2}, 0$ as geometric element and is thus of a different type to W (*cf.* Table 1.5.4.1).

In an *I*-centred lattice, the composition of W with the centring translation $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ has intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and location part $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$. One has $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, hence the symmetry operation $W' = y+\frac{1}{2}, x+\frac{1}{2}, \bar{z}+\frac{1}{2}$ is a screw rotation 2 $(\frac{1}{2}, \frac{1}{2}, 0)$ $x, x, \frac{1}{4}$ with the line $x, x, \frac{1}{4}$ as geometric element and is thus of a different type to W.

On the other hand, the translation subgroup $\mathcal{T}$ also contains the translation $t(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2})$. In this case, the intrinsic translation part of $W' = y+\frac{1}{2}, x-\frac{1}{2}, \bar{z}+\frac{1}{2}$ is $\boldsymbol{w}'_g = \boldsymbol{o}$, hence W' is of the same type as W, *i.e.* a twofold rotation. The location part is $\boldsymbol{w}'_l = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$ and since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{4} \end{pmatrix}$, the geometric element of W' is the line $x+\frac{1}{2}, x, \frac{1}{4}$.

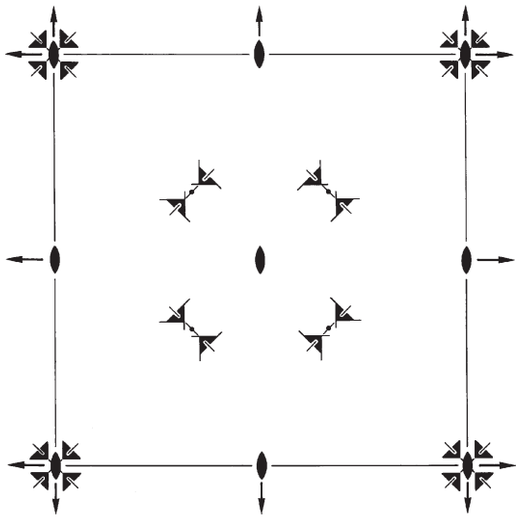


Figure 1.5.4.1
Symmetry-element diagram for space group $P23$ (195).

The analysis illustrates that the combination of the twofold rotation $2\ x, x, 0$ with I-centring translations gives rise to symmetry elements of rotation and of screw rotation type (*cf.* Table 1.5.4.2).

Example 5

Let $W = x, y, \bar{z}$ be a reflection $m\ x, y, 0$ with the c axis normal to the reflection plane. An F-centred lattice contains a centring translation $t(\frac{1}{2}, \frac{1}{2}, 0)$ and the composition of W with this translation is an n glide, since the intrinsic translation part of $W' = x + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$ is $\boldsymbol{w}'_g = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$ and consequently the location part is $\boldsymbol{w}'_l = \boldsymbol{o}$. The symmetry operation W' is thus an n glide with the plane $x, y, 0$ as geometric element. However, since the intrinsic translation part $\boldsymbol{w}_g$ is a lattice vector, W and W' are coplanar equivalents and belong to the element set of the same symmetry element, which is a reflection plane.

The composition of $W = x, y, \bar{z}$ with $t(0, \frac{1}{2}, \frac{1}{2})$ is a b glide, because $W' = x, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ has intrinsic translation part $\boldsymbol{w}'_g = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix}$. The location part is $\boldsymbol{w}'_l = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$ and since $(\boldsymbol{I} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{w}'_l$ for $\boldsymbol{p} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$, the geometric element of this glide reflection is the plane $x, y, \frac{1}{4}$. Likewise, the composition $W' = x + \frac{1}{2}, y, \bar{z} + \frac{1}{2}$ of W with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an a glide with the same plane $x, y, \frac{1}{4}$ as geometric element. The two symmetry operations $b\ x, y, \frac{1}{4}$ and $a\ x, y, \frac{1}{4}$, differing only by the lattice vector $(-\frac{1}{2}, \frac{1}{2}, 0)$ in their translation parts, are coplanar equivalents and belong to the element set of an e-glide plane (*cf.* Section 1.2.3 for an introduction to e-glide notation).

1.5.4.2. Synoptic table of the plane groups

The possible plane-group symbols are listed in Table 1.5.4.3. Two cases of multiple cells are included in addition to the standard cells, namely the c centring in the square system and the h centring in the hexagonal system. The c centring is defined by

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b};\ \ \mathbf{b}' = \pm\mathbf{a} + \mathbf{b}$$

with centring points at 0, 0 and $\frac{1}{2}, \frac{1}{2}$. The triple h cell is defined by

$$\mathbf{a}' = \mathbf{a} - \mathbf{b};\ \ \mathbf{b}' = \mathbf{a} + 2\mathbf{b}$$

with centring points at 0, 0; $\frac{2}{3}, \frac{1}{3}$ and $\frac{1}{3}, \frac{2}{3}$. The glide lines g directly listed under the mirror lines m in the extended and multiple cell symbols indicate that the two symmetry elements are parallel and alternate in the perpendicular direction.

1.5.4.3. Synoptic table of the space groups

Table 1.5.4.4 gives a comprehensive listing of the possible space-group symbols for various settings and choices of the unit cell. The data are ordered according to the crystal systems. The extended Hermann–Mauguin symbols provide information on the additional symmetry operations generated by the compositions of the symmetry operations with lattice translations. An extended Hermann–Mauguin symbol is a complex multi-line symbol: (i) the first line contains those symmetry operations for which the coordinate triplets are explicitly printed under 'Positions' in the space-group tables in this volume; (ii) the entries of the lines below indicate the additional symmetry operations generated by the compositions of the symmetry operations of the first line with lattice translations. For example, for A-, B-, C- and I-centred space groups, the entries of the second line of the two-line extended symbol denote the symmetry operations generated by combinations with the corresponding centring translations.[3]

In the triclinic system the corresponding symbols do not depend on any space direction. Therefore, only the two standard symbols $P1$ (1) and $P\bar{1}$ (2) are listed. One should, however, bear in mind that in some circumstances it might be more appropriate to use a centred cell for comparison purposes, *e.g.* following a phase transition resulting from a temperature, pressure or composition change.

The monoclinic and orthorhombic systems present the largest number of alternatives owing to various settings and cell choices. In the monoclinic system, three choices of unique axis can occur, namely b, c and a. In each case, two permutations of the other axes are possible, thus yielding six possible settings given in terms of three pairs, namely **ab**$\underline{\mathbf{c}}$ and **cb**$\underline{\bar{\mathbf{a}}}$, **ab**$\underline{\bar{\mathbf{c}}}$ and **ba**$\underline{\mathbf{c}}$, $\underline{\mathbf{a}}$**bc** and $\underline{\bar{\mathbf{a}}}$**cb**. The unique axes are underlined and the negative sign, placed over the letter, maintains the correct handedness of the reference system. The three possible cell choices indicated in Fig. 1.5.3.1 increase the number of possible symbols by a factor of three, thus yielding 18 different cases for each monoclinic space group, except for five cases, namely $P2$ (3), $P2_1$ (4), Pm (6), $P2/m$ (10) and $P2_1/m$ (11) with only six variants.

In monoclinic P lattices, the symmetry operations along the symmetry direction are always unique. Here again, as in the plane groups, the cell centrings give rise to additional entries in the extended Hermann–Mauguin symbols. Consider, for example, the data for monoclinic $P12/m1$ (10), $C12/m1$ (12) and $C12/c1$ (15) in Table 1.5.4.4. For $P12/m1$ and its various settings there is only one line, which corresponds to the full Hermann–Mauguin symbols; these contain only rotations 2 and reflections m. The first line for $C12/m1$ is followed by a second line, the first entry of which is the symbol $2_1/a$, because 2_1 screw rotations and a glide reflections also belong to this space group. Similarly, in $C12/c1$

[3] After the introduction of the e-glide convention and the symmetry-element interpretation of the characters of the Hermann–Mauguin symbols (de Wolff *et al.*, 1992), the tabulated data for the extended symbols were partially modified by introducing the e-glide notation in the symbols of only some of the groups [*cf.* Table 4.3.2.1 of the fifth edition of *IT* A (2002)]. In contrast to the fifth edition, in Table 1.5.4.4 extended symbols similar to those that can be found in the first four editions of *IT* A have been reinstated.

Table 1.5.4.3
List of plane-group symbols

System and lattice symbol	Point group	No. of plane group	Hermann–Mauguin symbol			Full symbol for other setting	Multiple cell
			Short	Full	Extended		
Oblique *p*	1 2	1 2		*p*1 *p*2			
Rectangular *p*, *c*	*m*	3 4 5	*pm* *pg* *cm*	*p*1*m*1 *p*1*g*1 *c*1*m*1	 *c*1*m*1 *g*	*p*11*m* *p*11*g* *c*11*m*	
	2*mm*	6 7 8 9		*p*2*mm* *p*2*mg* *p*2*gg* *c*2*mm*	 *c*2*mm* *g g*	*p*2*mm* *p*2*gm* *p*2*gg* *c*2*mm*	
Square *p*	4 4*mm*	10 11 12		*p*4 *p*4*mm* *p*4*gm*	 *p*4*mm* *g* *p*4*gm* *g*		*c*4 *c*4*mm* *g* *c*4*mg* *g*
Hexagonal *p*	3 3*m*	13 14 15		*p*3 *p*3*m*1 *p*31*m*	 *p*3*m*1 *g* *p*31*m* *g*		*h*3 *h*31*m* *g* *h*3*m*1 *g*
	6 6*mm*	16 17		*p*6 *p*6*mm*	 *p*6*mm* *g g*		*h*6 *h*6*mm* *g g*

rotations 2 and screw rotations 2_1 and *c* and *n* glide reflections alternate, and thus under the full symbol $C12/c1$ one finds the entry $2_1/n$.

In Table 1.5.4.4 the Hermann–Mauguin symbols of the orthorhombic space groups are listed in six different settings: the *standard setting* **abc**, and the settings **ba$\bar{\mathbf{c}}$**, **cab**, **$\bar{\mathbf{c}}$ba**, **bca** and **ac$\bar{\mathbf{b}}$**. These six settings result from the possible permutations of the three axes. Let us compare for a few space groups the standard setting **abc** with the **cab** setting. For *Pmm*2 (25) the permutation yields the new setting *P*2*mm*, reflecting the fact that the twofold axes parallel to the *c* direction change to the *a* direction. The mirrors normal to **a** and **b** become normal to **b** and **c**, respectively.

The case of *Cmm*2 (35) is slightly more complex due to the centring. As a result of the permutation the *C* centring becomes an *A* centring. The changes in the twofold axes and mirrors are similar to those of the previous example and result in the *A*2*mm* setting of *Cmm*2.

The extended Hermann–Mauguin symbol of the centred space group *Aem*2 (39) reveals the nature of the *e*-glide plane (also called the 'double' glide plane): among the set of glide reflections through the same (100) plane, there exist two glide reflections with glide components $\frac{1}{2}$**b** and $\frac{1}{2}$**c** (for details of the *e*-glide notation the reader is referred to Section 1.2.3, see also de Wolff *et al.*, 1992). In the **cab** setting, the *A* centring changes to a *B* centring and the double glide plane is now normal to **b** and the glide reflections have glide components $\frac{1}{2}$**a** and $\frac{1}{2}$**c**. The corresponding symbol is thus *B*2*em*. Note that in the cases of the five orthorhombic space groups whose Hermann–Mauguin symbols contain the *e*-glide symbol, namely *Aem*2 (39), *Aea*2 (41), *Cmce* (64), *Cmme* (67) and *Ccce* (68), the characters in the first lines of the extended symbols differ from the short symbols because the characters in the extended symbol represent symmetry operations, whereas those in the short and full symbol represent symmetry elements. In all these cases, the extended symbols listed in Table 1.5.4.4 are complemented by the short symbols, given in brackets.

The general discussion in Section 1.5.4.1 about the additional symmetry operations that occur as a result of combinations with lattice translations provides some rules for the construction of the extended Hermann–Mauguin symbols in the orthorhombic crystal system. In orthorhombic space groups with primitive lattices, the symmetry operations of any symmetry direction are always unique: either 2 or 2_1, either *m* or *a* or *b* or *c* or *n*. In *C*-centred lattices, owing to the possible combination of the original symmetry operations with the centring translations, the axes 2 along [100] and [010] alternate with axes 2_1. However, parallel to **c** there are either 2 or 2_1 axes because the combination of a rotation or screw rotation with a centring translation results in another operation of the same kind. Similarly, m_{100} alternates with b_{100}, m_{010} with a_{010}, c_{100} with n_{100} *etc.* The m_{001} reflection plane is simultaneously an n_{001} glide plane and an a_{001} glide plane is simultaneously a b_{001} glide plane. This latter plane with its double role is the e_{001} glide plane, as found for example in the full symbol of $C2/m\,2/m\,2/e$ (67) and the corresponding short symbol *Cmme*. As another example, consider the space group $C2/m\,2/c\,2_1/m$ (63). In Table 1.5.4.4, in the line of various settings for this space group the short Hermann–Mauguin symbols are listed, and the rotations or screw rotations do not appear. The m_{100}, c_{010} and m_{001} reflections and glide reflections occur alternating with b_{100}, n_{010} and n_{001} glide reflections, respectively. The entry under *Cmcm* is thus *bnn*.

F and *I* centring cause alternating symmetry operations for all three coordinate axes *a*, *b* and *c*. For these centrings, the permutation of the axes does not affect the symbol *F* or *I* of the centring type. However, the number of symmetry operations increases by a factor of four for *F* centrings and by a factor of two for *I* centrings when compared to those of a space group with a

(*continued on page* 106)

Table 1.5.4.4
List of space-group symbols for various settings and cells

TRICLINIC SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbol for all settings of the same unit cell
1	C_1^1	$P1$
2	C_i^1	$P\bar{1}$

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						
			abc	**cb̄a**	**abc̲**	**bac̄**	**a̲bc**	**ā̲cb**	Unique axis b Unique axis c Unique axis a
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121_1$	$A121_1$	$A112_1$	$B112_1$	$B211_1$	$C211_1$	Cell choice 1
			$A121_1$	$C121_1$	$B112_1$	$A112_1$	$C211_1$	$B211_1$	Cell choice 2
			$I121_1$	$I121_1$	$I112_1$	$I112_1$	$I211_1$	$I211_1$	Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$	$P1a1$	$P11a$	$P11b$	$Pb11$	$Pc11$	Cell choice 1
			$P1n1$	$P1n1$	$P11n$	$P11n$	$Pn11$	$Pn11$	Cell choice 2
			$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3
8	C_s^3	Cm	$C1m1$	$A1m1$	$A11m$	$B11m$	$Bm11$	$Cm11$	Cell choice 1
			$A1m1$	$C1m1$	$B11m$	$A11m$	$Cm11$	$Bm11$	Cell choice 2
			$I1m1$	$I1m1$	$I11m$	$I11m$	$Im11$	$Im11$	Cell choice 3
9	C_s^4	Cc	$C1c1$	$A1a1$	$A11a$	$B11b$	$Bb11$	$Cc11$	Cell choice 1
			$A1n1$	$C1n1$	$B11n$	$A11n$	$Cn11$	$Bn11$	Cell choice 2
			$I1a1$	$I1c1$	$I11b$	$I11a$	$Ic11$	$Ib11$	Cell choice 3
10	C_{2h}^1	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	C_{2h}^2	$P2_1/m$	$P1\frac{2_1}{m}1$	$P1\frac{2_1}{m}1$	$P11\frac{2_1}{m}$	$P11\frac{2_1}{m}$	$P\frac{2_1}{m}11$	$P\frac{2_1}{m}11$	
12	C_{2h}^3	$C2/m$	$C1\frac{2}{m}1$	$A1\frac{2}{m}1$	$A11\frac{2}{m}$	$B11\frac{2}{m}$	$B\frac{2}{m}11$	$C\frac{2}{m}11$	Cell choice 1
			$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	
			$A1\frac{2}{m}1$	$C1\frac{2}{m}1$	$B11\frac{2}{m}$	$A11\frac{2}{m}$	$C\frac{2}{m}11$	$B\frac{2}{m}11$	Cell choice 2
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$	
			$I1\frac{2}{m}1$	$I1\frac{2}{m}1$	$I11\frac{2}{m}$	$I11\frac{2}{m}$	$I\frac{2}{m}11$	$I\frac{2}{m}11$	Cell choice 3
			$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	
13	C_{2h}^4	$P2/c$	$P1\frac{2}{c}1$	$P1\frac{2}{a}1$	$P11\frac{2}{a}$	$P11\frac{2}{b}$	$P\frac{2}{b}11$	$P\frac{2}{c}11$	Cell choice 1
			$P1\frac{2}{n}1$	$P1\frac{2}{n}1$	$P11\frac{2}{n}$	$P11\frac{2}{n}$	$P\frac{2}{n}11$	$P\frac{2}{n}11$	Cell choice 2
			$P1\frac{2}{a}1$	$P1\frac{2}{c}1$	$P11\frac{2}{b}$	$P11\frac{2}{a}$	$P\frac{2}{c}11$	$P\frac{2}{b}11$	Cell choice 3

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						
			a$\underline{\mathbf{b}}$**c**	**c**$\bar{\mathbf{b}}$**a**	**ab**$\underline{\mathbf{c}}$	**ba**$\bar{\underline{\mathbf{c}}}$	$\underline{\mathbf{a}}$**bc**	$\bar{\underline{\mathbf{a}}}$**cb**	Unique axis *b* Unique axis *c* Unique axis *a*
14	C_{2h}^5	$P2_1/c$	$P1\frac{2_1}{c}1$	$P1\frac{2_1}{a}1$	$P11\frac{2_1}{a}$	$P11\frac{2_1}{b}$	$P\frac{2_1}{b}11$	$P\frac{2_1}{c}11$	Cell choice 1
			$P1\frac{2_1}{n}1$	$P1\frac{2_1}{n}1$	$P11\frac{2_1}{n}$	$P11\frac{2_1}{n}$	$P\frac{2_1}{n}11$	$P\frac{2_1}{n}11$	Cell choice 2
			$P1\frac{2_1}{a}1$	$P1\frac{2_1}{c}1$	$P11\frac{2_1}{b}$	$P11\frac{2_1}{a}$	$P\frac{2_1}{c}11$	$P\frac{2_1}{b}11$	Cell choice 3
15	C_{2h}^6	$C2/c$	$C1\frac{2}{c}1$	$A1\frac{2}{a}1$	$A11\frac{2}{a}$	$B11\frac{2}{b}$	$B\frac{2}{b}11$	$C\frac{2}{c}11$	Cell choice 1
			$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	$\frac{2_1}{n}$	
			$A1\frac{2}{n}1$	$C1\frac{2}{n}1$	$B11\frac{2}{n}$	$A11\frac{2}{n}$	$C\frac{2}{n}11$	$B\frac{2}{n}11$	Cell choice 2
			$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	$\frac{2_1}{a}$	$\frac{2_1}{c}$	$\frac{2_1}{b}$	
			$I1\frac{2}{a}1$	$I1\frac{2}{c}1$	$I11\frac{2}{b}$	$I11\frac{2}{a}$	$I\frac{2}{c}11$	$I\frac{2}{b}11$	Cell choice 3
			$\frac{2_1}{c}$	$\frac{2_1}{a}$	$\frac{2_1}{a}$	$\frac{2_1}{b}$	$\frac{2_1}{b}$	$\frac{2_1}{c}$	

ORTHORHOMBIC SYSTEM

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**bac̄**	**cab**	**c̄ba**	**bca**	**ac̄b**
16	D_2^1	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$
17	D_2^2	$P222_1$	$P222_1$	$P222_1$	$P2_122$	$P2_122$	$P22_12$	$P22_12$
18	D_2^3	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P22_12_1$	$P22_12_1$	$P2_122_1$	$P2_122_1$
19	D_2^4	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
20	D_2^5	$C222_1$	$C222_1$ $2_12_12_1$	$C222_1$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$B22_12$ $2_12_12_1$	$B22_12$ $2_12_12_1$
21	D_2^6	$C222$	$C222$ 2_12_12	$C222$ 2_12_12	$A222$ 22_12_1	$A222$ 22_12_1	$B222$ 2_122_1	$B222$ 2_122_1
22	D_2^7	$F222$	$F222$ 2_12_12 22_12_1 2_122_1	$F222$ 2_12_12 2_122_1 22_12_1	$F222$ 22_12_1 2_122_1 2_12_12	$F222$ 22_12_1 2_12_12 2_122_1	$F222$ 2_122_1 2_12_12 22_12_1	$F222$ 2_122_1 22_12_1 2_12_12
23	D_2^8	$I222$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$
24	D_2^9	$I2_12_12_1$	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222
25	C_{2v}^1	$Pmm2$	$Pmm2$	$Pmm2$	$P2mm$	$P2mm$	$Pm2m$	$Pm2m$
26	C_{2v}^2	$Pmc2_1$	$Pmc2_1$	$Pcm2_1$	$P2_1ma$	$P2_1am$	$Pb2_1m$	$Pm2_1b$
27	C_{2v}^3	$Pcc2$	$Pcc2$	$Pcc2$	$P2aa$	$P2aa$	$Pb2b$	$Pb2b$
28	C_{2v}^4	$Pma2$	$Pma2$	$Pbm2$	$P2mb$	$P2cm$	$Pc2m$	$Pm2a$
29	C_{2v}^5	$Pca2_1$	$Pca2_1$	$Pbc2_1$	$P2_1ab$	$P2_1ca$	$Pc2_1b$	$Pb2_1a$
30	C_{2v}^6	$Pnc2$	$Pnc2$	$Pcn2$	$P2na$	$P2an$	$Pb2n$	$Pn2b$
31	C_{2v}^7	$Pmn2_1$	$Pmn2_1$	$Pnm2_1$	$P2_1mn$	$P2_1nm$	$Pn2_1m$	$Pm2_1n$
32	C_{2v}^8	$Pba2$	$Pba2$	$Pba2$	$P2cb$	$P2cb$	$Pc2a$	$Pc2a$
33	C_{2v}^9	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$
34	C_{2v}^{10}	$Pnn2$	$Pnn2$	$Pnn2$	$P2nn$	$P2nn$	$Pn2n$	$Pn2n$
35	C_{2v}^{11}	$Cmm2$	$Cmm2$ $ba2$	$Cmm2$ $ba2$	$A2mm$ $2cb$	$A2mm$ $2cb$	$Bm2m$ $c2a$	$Bm2m$ $c2a$

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**bac̄**	**cab**	**c̄ba**	**bca**	**ac̄b**
36	C_{2v}^{12}	$Cmc2_1$	$Cmc2_1$ $bn2_1$	$Ccm2_1$ $na2_1$	$A2_1ma$ 2_1cn	$A2_1am$ 2_1nb	$Bb2_1m$ $n2_1a$	$Bm2_1b$ $c2_1n$
37	C_{2v}^{13}	$Ccc2$	$Ccc2$ $nn2$	$Ccc2$ $nn2$	$A2aa$ $2nn$	$A2aa$ $2nn$	$Bb2b$ $n2n$	$Bb2b$ $n2n$
38	C_{2v}^{14}	$Amm2$	$Amm2$ $nc2_1$	$Bmm2$ $cn2_1$	$B2mm$ 2_1na	$C2mm$ 2_1an	$Cm2m$ $b2_1n$	$Am2m$ $n2_1b$
39†	C_{2v}^{15}	$Aem2$	$Abm2$ ($Aem2$) $cc2_1$	$Bma2$ ($Bme2$) $cc2_1$	$B2cm$ ($B2em$) 2_1aa	$C2mb$ ($C2me$) 2_1aa	$Cm2a$ ($Cm2e$) $b2_1b$	$Ac2m$ ($Ae2m$) $b2_1b$
40	C_{2v}^{16}	$Ama2$	$Ama2$ $nn2_1$	$Bbm2$ $nn2_1$	$B2mb$ 2_1nn	$C2cm$ 2_1nn	$Cc2m$ $n2_1n$	$Am2a$ $n2_1n$
41†	C_{2v}^{17}	$Aea2$	$Aba2$ ($Aea2$) $cn2_1$	$Bba2$ ($Bbe2$) $nc2_1$	$B2cb$ ($B2eb$) 2_1an	$C2cb$ ($C2ce$) 2_1na	$Cc2a$ ($Cc2e$) $n2_1b$	$Ac2a$ ($Ae2a$) $b2_1n$
42	C_{2v}^{18}	$Fmm2$	$Fmm2$ $ba2$ $nc2_1$ $cn2_1$	$Fmm2$ $ba2$ $cn2_1$ $nc2_1$	$F2mm$ $2cb$ 2_1na 2_1an	$F2mm$ $2cb$ 2_1an 2_1na	$Fm2m$ $c2a$ $b2_1n$ $n2_1b$	$Fm2m$ $c2a$ $n2_1b$ $b2_1n$
43	C_{2v}^{19}	$Fdd2$	$Fdd2$ $dd2_1$	$Fdd2$ $dd2_1$	$F2dd$ 2_1dd	$F2dd$ 2_1dd	$Fd2d$ $d2_1d$	$Fd2d$ $d2_1d$
44	C_{2v}^{20}	$Imm2$	$Imm2$ $nn2_1$	$Imm2$ $nn2_1$	$I2mm$ 2_1nn	$I2mm$ 2_1nn	$Im2m$ $n2_1n$	$Im2m$ $n2_1n$
45	C_{2v}^{21}	$Iba2$	$Iba2$ $cc2_1$	$Iba2$ $cc2_1$	$I2cb$ 2_1aa	$I2cb$ 2_1aa	$Ic2a$ $b2_1b$	$Ic2a$ $b2_1b$
46	C_{2v}^{22}	$Ima2$	$Ima2$ $nc2_1$	$Ibm2$ $cn2_1$	$I2mb$ 2_1na	$I2cm$ 2_1an	$Ic2m$ $b2_1n$	$Im2a$ $n2_1b$
47	D_{2h}^{1}	$P\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$	$Pmmm$
48	D_{2h}^{2}	$P\frac{2}{n}\frac{2}{n}\frac{2}{n}$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$	$Pnnn$
49	D_{2h}^{3}	$P\frac{2}{c}\frac{2}{c}\frac{2}{m}$	$Pccm$	$Pccm$	$Pmaa$	$Pmaa$	$Pbmb$	$Pbmb$
50	D_{2h}^{4}	$P\frac{2}{b}\frac{2}{a}\frac{2}{n}$	$Pban$	$Pban$	$Pncb$	$Pncb$	$Pcna$	$Pcna$
51	D_{2h}^{5}	$P\frac{2_1}{m}\frac{2}{m}\frac{2}{a}$	$Pmma$	$Pmmb$	$Pbmm$	$Pcmm$	$Pmcm$	$Pmam$
52	D_{2h}^{6}	$P\frac{2}{n}\frac{2_1}{n}\frac{2}{a}$	$Pnna$	$Pnnb$	$Pbnn$	$Pcnn$	$Pncn$	$Pnan$
53	D_{2h}^{7}	$P\frac{2}{m}\frac{2}{n}\frac{2_1}{a}$	$Pmna$	$Pnmb$	$Pbmn$	$Pcnm$	$Pncm$	$Pman$
54	D_{2h}^{8}	$P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$	$Pcca$	$Pccb$	$Pbaa$	$Pcaa$	$Pbcb$	$Pbab$
55	D_{2h}^{9}	$P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$	$Pbam$	$Pbam$	$Pmcb$	$Pmcb$	$Pcma$	$Pcma$
56	D_{2h}^{10}	$P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$	$Pccn$	$Pccn$	$Pnaa$	$Pnaa$	$Pbnb$	$Pbnb$
57	D_{2h}^{11}	$P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}$	$Pbcm$	$Pcam$	$Pmca$	$Pmab$	$Pbma$	$Pcmb$
58	D_{2h}^{12}	$P\frac{2_1}{n}\frac{2_1}{n}\frac{2}{m}$	$Pnnm$	$Pnnm$	$Pmnn$	$Pmnn$	$Pnmn$	$Pnmn$
59	D_{2h}^{13}	$P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}$	$Pmmn$	$Pmmn$	$Pnmm$	$Pnmm$	$Pmnm$	$Pmnm$
60	D_{2h}^{14}	$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$	$Pbcn$	$Pcan$	$Pnca$	$Pnab$	$Pbna$	$Pcnb$
61	D_{2h}^{15}	$P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	$Pbca$	$Pcab$	$Pbca$	$Pcab$	$Pbca$	$Pcab$
62	D_{2h}^{16}	$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	$Pnma$	$Pmnb$	$Pbnm$	$Pcmn$	$Pmcn$	$Pnam$
63	D_{2h}^{17}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{m}$	$Cmcm$ bnn	$Ccmm$ nan	$Amma$ ncn	$Amam$ nnb	$Bbmm$ nna	$Bmmb$ cnn
64†	D_{2h}^{18}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{e}$	$Cmca$ ($Cmce$) bnb	$Ccmb$ ($Ccme$) naa	$Abma$ ($Aema$) ccn	$Acam$ ($Aeam$) bnb	$Bbcm$ ($Bbem$) naa	$Bmab$ ($Bmeb$) cnn

Table 1.5.4.4 (continued)

No. of space group	Schoen-flies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**bac̄**	**cab**	**c̄ba**	**bca**	**ac̄b**
65	D_{2h}^{19}	$C\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Cmmm* *ban*	*Cmmm* *ban*	*Ammm* *ncb*	*Ammm* *ncb*	*Bmmm* *cna*	*Bmmm* *cna*
66	D_{2h}^{20}	$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Cccm* *nnn*	*Cccm* *nnn*	*Amaa* *nnn*	*Amaa* *nnn*	*Bbmb* *nnn*	*Bbmb* *nnn*
67†	D_{2h}^{21}	$C\frac{2}{m}\frac{2}{m}\frac{2}{e}$	*Cmma* (*Cmme*) *bab*	*Cmmb* (*Cmme*) *baa*	*Abmm* (*Aemm*) *ccb*	*Acmm* (*Aemm*) *bcb*	*Bmcm* (*Bmem*) *caa*	*Bmam* (*Bmem*) *cca*
68†	D_{2h}^{22}	$C\frac{2}{c}\frac{2}{c}\frac{2}{e}$	*Ccca* (*Ccce*) *nnb*	*Cccb* (*Ccce*) *nna*	*Abaa* (*Aeaa*) *cnn*	*Acaa* (*Aeaa*) *bnn*	*Bbcb* (*Bbeb*) *nan*	*Bbab* (*Bbeb*) *ncn*
69	D_{2h}^{23}	$F\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Fmmm* *ban* *ncb* *cna*	*Fmmm* *ban* *cna* *ncb*	*Fmmm* *ncb* *cna* *ban*	*Fmmm* *ncb* *ban* *cna*	*Fmmm* *cna* *ban* *ncb*	*Fmmm* *cna* *ncb* *ban*
70	D_{2h}^{24}	$F\frac{2}{d}\frac{2}{d}\frac{2}{d}$	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*
71	D_{2h}^{25}	$I\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*
72	D_{2h}^{26}	$I\frac{2}{b}\frac{2}{a}\frac{2}{m}$	*I bam* *ccn*	*I bam* *ccn*	*I mcb* *naa*	*I mcb* *naa*	*I cma* *bnb*	*I cma* *bnb*
73	D_{2h}^{27}	$I\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*
74	D_{2h}^{28}	$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}$	*I mma* *nnb*	*I mmb* *nna*	*I bmm* *cnn*	*I cmm* *bnn*	*I mcm* *nan*	*I mam* *ncn*

† For the five space groups *Aem*2 (39), *Aea*2 (41), *Cmce* (64), *Cmme* (67) and *Ccce* (68), the 'new' space-group symbols, containing the symbol '*e*' for the 'double' glide plane, are given for all settings. These symbols were first introduced in the fourth edition of this volume (1995). For further explanations, see Sections 1.2.3 and 2.1.2, and de Wolff *et al.* (1992).

TETRAGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell *P* or *I*		Multiple cell *C* or *F*	
		Short	Extended	Short	Extended
75	C_4^1	*P*4		*C*4	
76	C_4^2	$P4_1$		$C4_1$	
77	C_4^3	$P4_2$		$C4_2$	
78	C_4^4	$P4_3$		$C4_3$	
79	C_4^5	*I* 4	*I*4 4_2	*F*4	*F*4 4_2
80	C_4^6	$I\,4_1$	$I4_1$ 4_3	$F4_1$	$F4_1$ 4_3
81	S_4^1	$P\bar{4}$		$C\bar{4}$	
82	S_4^2	$I\bar{4}$		$F\bar{4}$	
83	C_{4h}^1	*P*4/*m*		*C*4/*m*	$C4_2/m$ *n*
84	C_{4h}^2	$P4_2/m$		$C4_2/m$	$C4_2/m$ *n*
85	C_{4h}^3	*P*4/*n*		*C*4/*e*	*C*4/*a* *b*
86	C_{4h}^4	$P4_2/n$		$C4_2/e$	$C4_2/a$ *b*
87	C_{4h}^5	*I* 4/*m*	*I*4/*m* $4_2/n$	*F*4/*m*	*F*4/*m* $4_2/a$
88	C_{4h}^6	$I\,4_1/a$	$I4_1/a$ $4_3/b$	$F4_1/d$	$F4_1/d$ $4_3/d$
89	D_4^1	*P*422	*P*422 2_1	*C*422	*C*422 2_1
90	D_4^2	$P42_12$	$P42_12$ 2_1	$C422_1$	$C422_1$ 2_1

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
91	D_4^3	$P4_122$	$P4_122$ 2_1	$C4_122$	$C4_122$ 2_1
92	D_4^4	$P4_12_12$	$P4_12_12$ 2_1	$C4_122_1$	$C4_122_1$ 2_1
93	D_4^5	$P4_222$	$P4_222$ 2_1	$C4_222$	$C4_222$ 2_1
94	D_4^6	$P4_22_12$	$P4_22_12$ 2_1	$C4_222_1$	$C4_222_1$ 2_1
95	D_4^7	$P4_322$	$P4_322$ 2_1	$C4_322$	$C4_322$ 2_1
96	D_4^8	$P4_32_12$	$P4_32_12$ 2_1	$C4_322_1$	$C4_322_1$ 2_1
97	D_4^9	$I422$	$I422$ $4_22_12_1$	$F422$	$F422$ $4_22_12_1$
98	D_4^{10}	$I4_122$	$I4_122$ $4_32_12_1$	$F4_122$	$F4_122$ $4_32_12_1$
99	C_{4v}^1	$P4mm$	$P4mm$ g	$C4mm$	$C4mm$ b
100	C_{4v}^2	$P4bm$	$P4bm$ g	$C4mg_1$	$C4mg_1$ b
101	C_{4v}^3	$P4_2cm$	$P4_2cm$ g	$C4_2mc$	$C4_2mc$ b
102	C_{4v}^4	$P4_2nm$	$P4_2nm$ g	$C4_2mg_2$	$C4_2mg_2$ b
103	C_{4v}^5	$P4cc$	$P4cc$ n	$C4cc$	$C4cc$ n
104	C_{4v}^6	$P4nc$	$P4nc$ n	$C4cg_2$	$C4cg_2$ n
105	C_{4v}^7	$P4_2mc$	$P4_2mc$ n	$C4_2cm$	$C4_2cm$ n
106	C_{4v}^8	$P4_2bc$	$P4_2bc$ n	$C4_2cg_1$	$C4_2cg_1$ n
107	C_{4v}^9	$I4mm$	$I4mm$ 4_2nc	$F4mm$	$F4mm$ 4_2cg_2
108	C_{4v}^{10}	$I4cm$	$I4cc$ 4_2bm	$F4mc$	$F4cc$ 4_2mg_1
109	C_{4v}^{11}	$I4_1md$	$I4_1md$ 4_1nd	$F4_1dm$	$F4_1dm$ 4_3dg_2
110	C_{4v}^{12}	$I4_1cd$	$I4_1cd$ 4_3bd	$F4_1dc$	$F4_1dc$ 4_3dg_1
111	D_{2d}^1	$P\bar{4}2m$	$P\bar{4}2m$ g	$C\bar{4}m2$	$C\bar{4}m2$ b
112	D_{2d}^2	$P\bar{4}2c$	$P\bar{4}2c$ n	$C\bar{4}c2$	$C\bar{4}c2$ n
113	D_{2d}^3	$P\bar{4}2_1m$	$P\bar{4}2_1m$ g	$C\bar{4}m2_1$	$C\bar{4}m2_1$ b
114	D_{2d}^4	$P\bar{4}2_1c$	$P\bar{4}2_1c$ n	$C\bar{4}c2_1$	$C\bar{4}c2_1$ n
115	D_{2d}^5	$P\bar{4}m2$	$P\bar{4}m2$ 2_1	$C\bar{4}2m$	$C\bar{4}2m$ 2_1
116	D_{2d}^6	$P\bar{4}c2$	$P\bar{4}c2$ 2_1	$C\bar{4}2c$	$C\bar{4}2c$ 2_1
117	D_{2d}^7	$P\bar{4}b2$	$P\bar{4}b2$ 2_1	$C\bar{4}2g_1$	$C\bar{4}2g_1$ 2_1
118	D_{2d}^8	$P\bar{4}n2$	$P\bar{4}n2$ 2_1	$C\bar{4}2g_2$	$C\bar{4}2g_2$ 2_1
119	D_{2d}^9	$I\bar{4}m2$	$I\bar{4}m2$ $n2_1$	$F\bar{4}2m$	$F\bar{4}2m$ 2_1g_2
120	D_{2d}^{10}	$I\bar{4}c2$	$I\bar{4}c2$ $b2_1$	$F\bar{4}2c$	$F\bar{4}2c$ 2_1n
121	D_{2d}^{11}	$I\bar{4}2m$	$I\bar{4}2m$ 2_1c	$F\bar{4}m2$	$F\bar{4}m2$ $c2_1$
122	D_{2d}^{12}	$I\bar{4}2d$	$I\bar{4}2d$ 2_1d	$F\bar{4}d2$	$F\bar{4}d2$ $d2_1$

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P or I		Multiple cell C or F	
		Short	Extended	Short	Extended
123	D_{4h}^1	$P4/mmm$	$P4/m\ 2/m\ 2/m$	$C4/mmm$	$C4/mmm$
			$2_1/g$		nb
124	D_{4h}^2	$P4/mcc$	$P4/m\ 2/c\ 2/c$	$C4/mcc$	$C4/mcc$
			$2_1/n$		nn
125	D_{4h}^3	$P4/nbm$	$P4/n\ 2/b\ 2/m$	$C4/emg_1$	$C4/amg_1$
			$2_1/g$		bb
126	D_{4h}^4	$P4/nnc$	$P4/n\ 2/n\ 2/c$	$C4/ecg_2$	$C4/acg_2$
			$2_1/n$		bn
127	D_{4h}^5	$P4/mbm$	$P4/m\ 2_1/b\ 2/m$	$C4/mmg_1$	$C4/mmg_1$
			$2_1/g$		nb
128	D_{4h}^6	$P4/mnc$	$P4/m\ 2_1/n\ 2/c$	$C4/mcg_2$	$C4/mcg_2$
			$2_1/n$		nn
129	D_{4h}^7	$P4/nmm$	$P4/n\ 2_1/m\ 2/m$	$C4/emm$	$C4amm$
			$2_1/g$		bb
130	D_{4h}^8	$P4/ncc$	$P4/n\ 2_1/c\ 2/c$	$C4/ecc$	$C4/acc$
			$2_1/n$		bn
131	D_{4h}^9	$P4_2/mmc$	$P4_2/m\ 2/m\ 2/c$	$C4_2/mcm$	$C4_2/mcm$
			$2_1/n$		nn
132	D_{4h}^{10}	$P4_2/mcm$	$P4_2/m\ 2/c\ 2/m$	$C4_2/mmc$	$C4_2/mmc$
			$2_1/g$		nb
133	D_{4h}^{11}	$P4_2/nbc$	$P4_2/n\ 2/b\ 2/c$	$C4_2/ecg_1$	$C4_2/acg_1$
			$2_1/n$		bn
134	D_{4h}^{12}	$P4_2/nnm$	$P4_2/n\ 2/n\ 2/m$	$C4_2/emg_2$	$C4_2/amg_2$
			$2_1/g$		bb
135	D_{4h}^{13}	$P4_2/mbc$	$P4_2/m\ 2_1/b\ 2/c$	$C4_2/mcg_1$	$C4_2/mcg_1$
			$2_1/n$		nn
136	D_{4h}^{14}	$P4_2/mnm$	$P4_2/m\ 2_1/n\ 2/m$	$C4_2/mmg_2$	$C4_2/mmg_2$
			$2_1/g$		nb
137	D_{4h}^{15}	$P4_2/nmc$	$P4_2/n\ 2_1/m\ 2/c$	$C4_2/ecm$	$C4_2/acm$
			$2_1/n$		bn
138	D_{4h}^{16}	$P4_2/ncm$	$P4_2/n\ 2_1/c\ 2/m$	$C4_2/emc$	$C4_2/amc$
			$2_1/g$		bb
139	D_{4h}^{17}	$I4/mmm$	$I4/m\ 2/m\ 2/m$	$F4/mmm$	$F4/mmm$
			$4_2/n\ 2_1/n\ 2_1/c$		$4_2/acg_2$
140	D_{4h}^{18}	$I4/mcm$	$I4/m\ \ 2/c\ \ 2/c$	$F4/mmc$	$F4/mcc$
			$4_2/n\ \ 2_1/b\ \ 2_1/m$		$4_2/amg_1$
141	D_{4h}^{19}	$I4_1/amd$	$I4_1/a\ \ 2/m\ \ 2/d$	$F4_1/ddm$	$F4_1/ddm$
			$4_3/b\ \ 2_1/n\ \ 2_1/d$		$4_3/ddg_2$
142	D_{4h}^{20}	$I4_1/acd$	$I4_1/a\ \ 2/c\ \ 2/d$	$F4_1/ddc$	$F4_1/ddc$
			$4_3/b\ \ 2_1/b\ \ 2_1/d$		$4_3/ddg_1$

Note: The glide planes g, g_1 and g_2 have the glide components $g(\frac{1}{2}, \frac{1}{2}, 0)$, $g_1(\frac{1}{4}, \frac{1}{4}, 0)$ and $g_2(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$. For the glide plane symbol 'e', see Sections 1.2.3 and 2.1.2, and de Wolff *et al.* (1992).

TRIGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P or R			Triple cell H
		Short	Full	Extended	
143	C_3^1	$P3$			$H3$
144	C_3^2	$P3_1$			$H3_1$
145	C_3^3	$P3_2$			$H3_2$
146	C_3^4	$R3$		$R3$	
				$3_{1,2}$	
147	C_{3i}^1	$P\bar{3}$			$H\bar{3}$
148	C_{3i}^2	$R\bar{3}$		$R\bar{3}$	
				$3_{1,2}$	
149	D_3^1	$P312$		$P312$	$H321$
				2_1	
150	D_3^2	$P321$		$P321$	$H312$
				2_1	
151	D_3^3	$P3_112$		$P3_112$	$H3_121$
				2_1	

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P or R			Triple cell H
		Short	Full	Extended	
152	D_3^4	$P3_121$		$P3_121$ 2_1	$H3_112$
153	D_3^5	$P3_212$		$P3_212$ 2_1	$H3_221$
154	D_3^6	$P3_221$		$P3_221$ 2_1	$H3_212$
155	D_3^7	$R32$		$R3\ 2$ $3_{1,2}2_1$	
156	C_{3v}^1	$P3m1$		$P3m1$ b	$H31m$
157	C_{3v}^2	$P31m$		$P31m$ a	$H3m1$
158	C_{3v}^3	$P3c1$		$P3c1$ n	$H31c$
159	C_{3v}^4	$P31c$		$P31c$ n	$H3c1$
160	C_{3v}^5	$R3m$		$R3\ m$ $3_{1,2}b$	
161	C_{3v}^6	$R3c$		$R3\ c$ $3_{1,2}n$	
162	D_{3d}^1	$P\bar{3}1m$	$P\bar{3}12/m$	$P\bar{3}12/m$ $2_1/a$	$H\bar{3}m1$
163	D_{3d}^2	$P\bar{3}1c$	$P\bar{3}12/c$	$P\bar{3}12/c$ $2_1/n$	$H\bar{3}c1$
164	D_{3d}^3	$P\bar{3}m1$	$P\bar{3}2/m1$	$P\bar{3}2/m1$ $2_1/b$	$H\bar{3}1m$
165	D_{3d}^4	$P\bar{3}c1$	$P\bar{3}2/c1$	$P\bar{3}2/c1$ $2_1/n$	$H\bar{3}1c$
166	D_{3d}^5	$R\bar{3}m$	$R\bar{3}2/m$	$R\bar{3}\ 2/m$ $3_{1,2}2_1/b$	
167	D_{3d}^6	$R\bar{3}c$	$R\bar{3}2/c$	$R\bar{3}\ 2/c$ $3_{1,2}2_1/n$	

HEXAGONAL SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell P			Triple cell H
		Short	Full	Extended	
168	C_6^1	$P6$			$H6$
169	C_6^2	$P6_1$			$H6_1$
170	C_6^3	$P6_5$			$H6_5$
171	C_6^4	$P6_2$			$H6_2$
172	C_6^5	$P6_4$			$H6_4$
173	C_6^6	$P6_3$			$H6_3$
174	C_{3h}^1	$P\bar{6}$			$H\bar{6}$
175	C_{6h}^1	$P6/m$			$H6/m$
176	C_{6h}^2	$P6_3/m$			$H6_3/m$
177	D_6^1	$P622$		$P62\ 2$ 2_12_1	$H622$
178	D_6^2	$P6_122$		$P6_12\ 2$ 2_12_1	$H6_122$
179	D_6^3	$P6_522$		$P6_52\ 2$ 2_12_1	$H6_522$
180	D_6^4	$P6_222$		$P6_22\ 2$ 2_12_1	$H6_222$
181	D_6^5	$P6_422$		$P6_42\ 2$ 2_12_1	$H6_422$
182	D_6^6	$P6_322$		$P6_32\ 2$ 2_12_1	$H6_322$

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols for standard cell *P*			Triple cell *H*
		Short	Full	Extended	
183	C_{6v}^1	*P*6*mm*		*P*6*mm* *b a*	*H*6*mm*
184	C_{6v}^2	*P*6*cc*		*P*6*cc* *nn*	*H*6*cc*
185	C_{6v}^3	$P6_3cm$		$P6_3cm$ *na*	$H6_3mc$
186	C_{6v}^4	$P6_3mc$		$P6_3mc$ *b n*	$H6_3cm$
187	D_{3h}^1	$P\bar{6}m2$		$P\bar{6}m2$ $b\,2_1$	$H\bar{6}2m$
188	D_{3h}^2	$P\bar{6}c2$		$P\bar{6}c2$ $n2_1$	$H\bar{6}2c$
189	D_{3h}^3	$P\bar{6}2m$		$P\bar{6}2m$ 2_1a	$H\bar{6}m2$
190	D_{3h}^4	$P\bar{6}2c$		$P\bar{6}2\ c$ 2_1n	$H\bar{6}c2$
191	D_{6h}^1	*P*6/*mmm*	*P*6/*m* 2/*m*2/*m*	*P*6/*m* 2/*m* 2/*m* $2_1/b$ $2_1/a$	*H*6/*mmm*
192	D_{6h}^2	*P*6/*mcc*	*P*6/*m* 2/*c* 2/*c*	*P*6/*m* 2/*c* 2/*c* $2_1/n$ $2_1/n$	*H*6/*mcc*
193	D_{6h}^3	$P6_3/mcm$	$P6_3/m\,2/c\,2/m$	$P6_3/m$ 2/*c* 2/*m* $2_1/b$ $2_1/a$	$H6_3/mmc$
194	D_{6h}^4	$P6_3/mmc$	$P6_3/m2/m2/c$	$P6_3/m$ 2/*m* 2/*c* $2_1/b$ $2_1/n$	$H6_3/mcm$

CUBIC SYSTEM

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols		
		Short	Full	Extended†
195	T^1	*P*23		
196	T^2	*F*23		*F*23 2 2_1 2_1
197	T^3	*I*23		*I*23 2_1
198	T^4	$P2_13$		
199	T^5	$I2_13$		$I2_13$ 2
200	T_h^1	$Pm\bar{3}$	$P2/m\,\bar{3}$	
201	T_h^2	$Pn\bar{3}$	$P2/n\,\bar{3}$	
202	T_h^3	$Fm\bar{3}$	$F2/m\,\bar{3}$	$F2/m\,\bar{3}$ 2/*n* $2_1/b$ $2_1/a$
203	T_h^4	$Fd\bar{3}$	$F2/d\,\bar{3}$	$F2/d\,\bar{3}$ 2/*d* $2_1/d$ $2_1/d$
204	T_h^5	$Im\bar{3}$	$I2/m\,\bar{3}$	$I2/m\,\bar{3}$ $2_1/n$
205	T_h^6	$Pa\bar{3}$‡	$P2_1/a\bar{3}$‡	
206	T_h^7	$Ia\bar{3}$	$I2_1/a\bar{3}$	$I2_1/a\,\bar{3}$ 2/*b*
207	O^1	*P*432		*P*432 2_1
208	O^2	$P4_232$		$P4_232$ 2_1

Table 1.5.4.4 (continued)

No. of space group	Schoenflies symbol	Hermann–Mauguin symbols		
		Short	Full	Extended†
209	O^3	$F432$		$F432$ 42 4_22_1 4_22_1
210	O^4	$F4_132$		$F4_132$ $4_1\ 2$ $4_3\ 2_1$ $4_3\ 2_1$
211	O^5	$I432$		$I432$ $4_2\ 2_1$
212	O^6	$P4_332$		$P4_332$ 2_1
213	O^7	$P4_132$		$P4_132$ 2_1
214	O^8	$I4_132$		$I4_132$ $4_3\ 2_1$
215	T_d^1	$P\bar{4}3m$		$P\bar{4}3m$ g
216	T_d^2	$F\bar{4}3m$		$F\bar{4}3m$ g g_2 g_2
217	T_d^3	$I\bar{4}3m$		$I\bar{4}3m$ n
218	T_d^4	$P\bar{4}3n$		$P\bar{4}3n$ c
219	T_d^5	$F\bar{4}3c$		$F\bar{4}3n$ c g_1 g_1
220	T_d^6	$I\bar{4}3d$		$I\bar{4}3d$ d
221	O_h^1	$Pm\bar{3}m$	$P4/m\,\bar{3}2/m$	$P4/m\,\bar{3}2/m$ $2_1/g$
222	O_h^2	$Pn\bar{3}n$	$P4/n\,\bar{3}2/n$	$P4/n\,\bar{3}2/n$ $2_1/c$
223	O_h^3	$Pm\bar{3}n$	$P4_2/m\bar{3}2/n$	$P4_2/m\bar{3}2/n$ $2_1/c$
224	O_h^4	$Pn\bar{3}m$	$P4_2/n\bar{3}2/m$	$P4_2/n\bar{3}2/m$ $2_1/g$
225	O_h^5	$Fm\bar{3}m$	$F4/m\,\bar{3}2/m$	$F4/m\,\bar{3}\,2/m$ $4/n\quad 2/g$ $4_2/b\quad 2_1/g_2$ $4_2/a\quad 2_1/g_2$
226	O_h^6	$Fm\bar{3}c$	$F4/m\,\bar{3}2/c$	$F4/m\bar{3}2/n$ $4/n\ \ 2/c$ $4_2/b\ \ 2_1/g_1$ $4_2/a\ \ 2_1/g_1$
227	O_h^7	$Fd\bar{3}m$	$F4_1/d\bar{3}2/m$	$F4_1/d\bar{3}2/m$ $4_1/d\ \ 2/g$ $4_3/d\ \ 2_1/g_2$ $4_3/d\ \ 2_1/g_2$
228	O_h^8	$Fd\bar{3}c$	$F4_1/d\bar{3}2/c$	$F4_1/d\bar{3}2/n$ $4_1/d\ \ 2/c$ $4_3/d\ \ 2_1/g_1$ $4_3/d\ \ 2_1/g_1$
229	O_h^9	$Im\bar{3}m$	$I4/m\,\bar{3}2/m$	$I4/m\bar{3}2/m$ $4_2/n\ 2_1/n$
230	O_h^{10}	$Ia\bar{3}d$	$I4_1/a\,\bar{3}2/d$	$I4_1/a\bar{3}2/d$ $4_3/b\ \ 2_1/d$

† Axes 3_1 and 3_2 parallel to axes 3 are not indicated in the extended symbols: *cf.* Section 1.5.4.1. ‡ The alternative setting $Pb\bar{3}$ ($P2_1/b\bar{3}$) of $Pa\bar{3}$ is of importance for diffraction studies, *cf.* Section 1.5.4.3 and Table 1.6.4.25. *Note:* The glide planes g, g_1 and g_2 have the glide components $g(\frac{1}{2},\frac{1}{2},0)$, $g_1(\frac{1}{4},\frac{1}{4},0)$ and $g_2(\frac{1}{4},\frac{1}{4},\frac{1}{2})$.

primitive lattice. In *Fmm*2 (42) for example, three additional lines appear in the extended symbol, namely $ba2$, $nc2_1$ and $cn2_1$. These operations are obtained by combining successively the centring translations $t(\frac{1}{2},\frac{1}{2},0)$, $t(0,\frac{1}{2},\frac{1}{2})$ and $t(\frac{1}{2},0,\frac{1}{2})$ with the symmetry operations of *Pmm*2. However, in space groups *Fdd*2 (43) and *Fddd* (70) the nature of the *d* planes is not altered by the translations of the *F*-centred lattice; for this reason, in Table 1.5.4.4 a two-line symbol for *Fdd*2 and a one-line symbol for *Fddd* are sufficient.

In tetragonal space groups with primitive lattices there are no alternating symmetry operations belonging to the symmetry directions [001] and [100]. However, for the symmetry direction $[1\bar{1}0]$ the symmetry operations 2 and 2_1 alternate, as do the reflection *m* and the glide reflection *g* [*g* is the name for a glide reflection with a glide vector $(\frac{1}{2},\frac{1}{2},0)$], and the glide reflections *c* and *n*. For example, the second line of the extended symbol of $P4_2/n\,2/b\,2/c$ (133) contains the expression $2_1/n$ under the expression $2/c$.

For the space groups in the tetragonal system, the unique axis is always the *c* axis, thus reducing the number of settings and choices of the unit cell. Two additional multiple cells are considered in this system, namely the *C* and *F* cells obtained from the *P* and *I* cell by the following relations:

$$\mathbf{a}' = \mathbf{a} \mp \mathbf{b};\ \ \mathbf{b}' = \pm\mathbf{a} + \mathbf{b};\ \ \mathbf{c}' = \mathbf{c}.$$

The secondary [100] and tertiary [110] symmetry directions are interchanged in this cell transformation. As an example, consider $P4/n$ (85) and its description with respect to a *C*-centred basis. Under the transformation $\mathbf{a}' = \mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, the *n* glide $n(\frac{1}{2},\frac{1}{2},0)$ $x, y, 0$ is transformed to an *a* glide a $x, y, 0$ while its coplanar equivalent glide $n(-\frac{1}{2},\frac{1}{2},0)$ $x, y, 0$ is transformed to a *b* glide b $x, y, 0$. Thus, the extended symbol of the multiple-cell description of $P4/n$ (85) shown in Table 1.5.4.4 is $C4/a(b)$, while in accordance with the *e*-glide convention, the short Hermann–Mauguin symbol becomes $C4/e$.

In the case of $I4/m$ (87), as a result of the *I* centring, screw rotations 4_2 and glide reflections *n* normal to 4_2 appear as additional symmetry operations and are shown in the second line of the extended symbol (*cf.* Table 1.5.4.4). In the multiple-cell setting, the space group $F4/m$ exhibits the additional fourfold screw axis 4_2 and owing to the new orientation of the a' and b' axes, which are rotated by 45° relative to the original axes *a* and *b*, the *n* glide of $I4/m$ becomes an *a* glide in the extended Hermann–Mauguin symbol. The additional *b* glide obtained from a coplanar *n* glide is not given explicitly in the extended symbol.

The rhombohedral space groups are listed together with the trigonal space groups under the heading 'Trigonal system'. For both representative symmetry directions $[001]_{\rm hex}$ and $[100]_{\rm hex}$, rotations with screw rotations and reflections with glide reflections or different kinds of glide reflections alternate, so that additional symmetry operations always occur: rotations 3 or rotoinversions $\bar{3}$ are accompanied by 3_1 and 3_2 screw rotations; 2 rotations alternate with 2_1 screw rotations and *m* reflections or *c* glide reflections alternate with additional glide reflections. As examples, under the full Hermann–Mauguin symbol $R3$ (146) one finds $3_{1,2}$ and in the line under $R\,\bar{3}\,2/c$ (167) one finds $3_{1,2}\ 2_1/n$.

The extended Hermann–Mauguin symbols for space groups of the hexagonal crystal system retain the symbol for the primary symmetry direction [001]. Along the secondary $\langle 100\rangle$ and tertiary $\langle 1\bar{1}0\rangle$ symmetry directions every horizontal axis 2 is accompanied by a screw rotation 2_1, while the reflections and glide reflections, or different types of glide reflections, alternate.

The list of hexagonal and trigonal space-group symbols is completed by a multiple *H* cell, which is three times the volume of the corresponding *P* cell. The unit-cell transformation is obtained from the relation

$$\mathbf{a}' = \mathbf{a} - \mathbf{b};\ \ \mathbf{b}' = \mathbf{a} + 2\mathbf{b};\ \ \mathbf{c}' = \mathbf{c}$$

with centring points at 0, 0, 0; $\frac{2}{3},\frac{1}{3},0$ and $\frac{1}{3},\frac{2}{3},0$. The new vectors $\mathbf{a}'$ and $\mathbf{b}'$ are rotated by −30° in the *ab* plane with respect to the old vectors **a** and **b**. There are altogether six possible such multiple cells rotated by ±30°, ±90° and ±150° (*cf.* Table 1.5.1.1 and Fig. 1.5.1.8).

The hexagonal lattice is frequently referred to the orthohexagonal *C*-centred cell (*cf.* Table 1.5.1.1 and Fig. 1.5.1.7). The volume of this centred cell is twice the volume of the primitive hexagonal cell and its basis vectors are mutually perpendicular.

In general, the space groups of the cubic system do not yield any additional orientations and only the short, full and extended symbols are given. The only exception to this general rule is the group $Pa\bar{3}$ (205) with its alternative setting $Pb\bar{3}$, whose basis vectors $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ are related by a rotation of 90° in the *ab* plane to the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ of $Pa\bar{3}$: $\mathbf{a}' = \mathbf{b}, \mathbf{b}' = -\mathbf{a}, \mathbf{c}' = \mathbf{c}$. The different general reflection conditions of $Pb\bar{3}$ in comparison to those of $Pa\bar{3}$ indicate its importance for diffraction studies (*cf.* Table 1.6.4.25). In some extended symbols of the cubic groups, we note the use of the *g* or g_i type of glide reflections as in, for example, $F\bar{4}3c$ (219). The *g* glide is a generic form of a glide plane which is different from the usual glide planes denoted by *a*, *b*, *c*, *n*, *d* or *e*. The symbols *g*, g_1 and g_2 indicate specific glide components and orientations that are specified in the *Note* to Table 1.5.4.4.

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1.6. Methods of space-group determination

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1.6.1. Overview

This chapter describes and discusses several methods of symmetry determination of single-domain crystals. A detailed presentation of symmetry determination from diffraction data is given in Section 1.6.2.1, followed by a brief discussion of intensity statistics, ideal as well as non-ideal, with an application of the latter to real intensity data from a $P\overline{1}$ crystal structure in Section 1.6.2.2. Several methods of retrieving symmetry information from a solved crystal structure are then discussed (Section 1.6.2.3). This is followed by a discussion of chemical and physical restrictions on space-group symmetry (Section 1.6.2.4), including some aids in symmetry determination, and by a brief section on pitfalls in space-group determination (Section 1.6.2.5).

The following two sections deal with reflection conditions. Section 1.6.3 presents the theoretical background of conditions for possible general reflections and their corresponding derivation. A brief discussion of special reflection conditions is included. Section 1.6.4 presents an extensive tabulation of general reflection conditions and possible space groups.

Other methods of space-group determination are presented in Section 1.6.5. Section 1.6.5.1 deals with an account of methods of space-group determination based on resonant (also termed 'anomalous') scattering. Section 1.6.5.2 is a brief description of approaches to space-group determination in macromolecular crystallography. Section 1.6.5.3 deals with corresponding approaches in powder-diffraction methods.

The chapter concludes with a description and illustration of symmetry determination based on electron-diffraction methods (Section 1.6.6), and principally focuses on convergent-beam electron diffraction.

This chapter deals only with single crystals. A supplement (Flack, 2015) deals with twinned crystals and those displaying a specialized metric.

1.6.2. Symmetry determination from single-crystal studies

By U. Shmueli and H. D. Flack

1.6.2.1. Symmetry information from the diffraction pattern

The extraction of symmetry information from the diffraction pattern takes place in three stages.

In the first stage, the unit-cell dimensions are determined and analyzed in order to establish to which Bravais lattice the crystal belongs. A conventional choice of lattice basis (coordinate system) may then be chosen. The determination of the Bravais lattice[1] of the crystal is achieved by the process of cell reduction, in which the lattice is first described by a basis leading to a primitive unit cell, and then linear combinations of the unit-cell vectors are taken to reduce the metric tensor (and the cell dimensions) to a standard form. From the relationships amongst the elements of the metric tensor, one obtains the Bravais lattice, together with a conventional choice of the unit cell, with the aid of standard tables. A detailed description of cell reduction is given in Chapter 3.1 of this volume and in Part 9 of earlier editions (*e.g.* Burzlaff *et al.*, 2002). An alternative approach (Le Page, 1982) seeks the Bravais lattice directly from the cell dimensions by searching for all the twofold axes present. All these operations are automated in software. Regardless of the technique employed, at the end of the process one obtains an indication of the Bravais lattice and a unit cell in a conventional setting for the crystal system, primitive or centred as appropriate. These are usually good indications which, however, must be confirmed by an examination of the distribution of diffracted intensities as outlined below.

In the second stage, it is the point-group symmetry of the intensities of the Bragg reflections which is determined. We recall that the average reduced intensity of a pair of Friedel opposites (hkl and $\overline{hkl}$) is given by

$$\begin{aligned}|F_{\rm av}(\mathbf{h})|^2 &= \tfrac{1}{2}[|F(\mathbf{h})|^2 + |F(\overline{\mathbf{h}})|^2] \\ &= \sum_{i,j}[(f_i + f_i')(f_j + f_j') + f_i'' f_j'']\cos[2\pi\mathbf{h}(\mathbf{r}_i - \mathbf{r}_j)] \equiv A(\mathbf{h}),\end{aligned} \tag{1.6.2.1}$$

where the atomic scattering factor of atom j, taking into account resonant scattering, is given by

$$\mathbf{f}_j = f_j + f_j' + if_j'',$$

the wavelength-dependent components f_j' and f_j'' being the real and imaginary parts, respectively, of the contribution of atom j to the resonant scattering, $\mathbf{h}$ contains in the (row) matrix (1×3) the diffraction orders (hkl) and $\mathbf{r}_j$ contains in the (column) matrix (3×1) the coordinates (x_j, y_j, z_j) of atom j. The components of the $\mathbf{f}_j$ are assumed to contain implicitly the displacement parameters. Equation (1.6.2.1) can be found *e.g.* in Okaya & Pepinsky (1955), Rossmann & Arnold (2001) and Flack & Shmueli (2007). It follows from (1.6.2.1) that

$$|F_{\rm av}(\mathbf{h})|^2 = |F_{\rm av}(\overline{\mathbf{h}})|^2 \text{ or } A(\mathbf{h}) = A(\overline{\mathbf{h}}),$$

regardless of the contribution of resonant scattering. Hence the averaging introduces a centre of symmetry in the (averaged) diffraction pattern.[2] In fact, working with the average of Friedel opposites, one may determine the Laue group of the diffraction pattern by comparing the intensities of reflections which should be symmetry equivalent under each of the Laue groups. These are the 11 centrosymmetric point groups: $\overline{1}$, $2/m$, mmm, $4/m$, $4/mmm$, $\overline{3}$, $\overline{3}m$, $6/m$, $6/mmm$, $m\overline{3}$ and $m\overline{3}m$. For example, the reflections of which the intensities are to be compared for the Laue group $\overline{3}$ are: hkl, kil, ihl, $\overline{hkl}$, $\overline{kil}$ and $\overline{ihl}$, where $i = -h - k$. An extensive listing of the indices of symmetry-related reflections in all the point groups, including of course the Laue groups, is

[1] The Bravais lattice symbol consists of two characters. The first is the first letter of the name of a crystal family and the second is the centring mode of a conventional unit cell. For details see Tables 3.1.2.1 and 3.1.2.2.

[2] We must mention the well known Friedel's law, which states that $|F(\mathbf{h})|^2 = |F(\overline{\mathbf{h}})|^2$ and which is only a reasonable approximation for noncentrosymmetric crystals if resonant scattering is negligibly small. This law holds well for centrosymmetric crystals, independently of the resonant-scattering contribution.

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given in Appendix 1.4.4 of *International Tables for Crystallography* Volume B (Shmueli, 2008).[3] In the past, one used to inspect the diffraction images to see which classes of reflections are symmetry equivalent within experimental and other uncertainty. Nowadays, the whole intensity data set is analyzed by software. The intensities are merged and averaged under each of the 11 Laue groups in various settings (*e.g.* 2/*m* unique axis *b* and unique axis *c*) and orientations (*e.g.* $\bar{3}m1$ and $\bar{3}1m$). For each choice of Laue group and its variant, an $R_{\rm merge}$ factor is calculated as follows:

$$R_{{\rm merge},i} = \frac{\sum_{\mathbf{h}} \sum_{s=1}^{|G|_i} |\langle |F_{\rm av}(\mathbf{h})|^2 \rangle_i - |F_{\rm av}(\mathbf{h}\boldsymbol{W}_{si})|^2|}{|G|_i \sum_{\mathbf{h}} \langle |F_{\rm av}(\mathbf{h})|^2 \rangle_i}, \qquad (1.6.2.2)$$

where $\boldsymbol{W}_{si}$ is the matrix of the *s*th symmetry operation of the *i*th Laue group, $|G_i|$ is the number of symmetry operations in that group, the average in the first term in the numerator and in the denominator ranges over the intensities of the trial Laue group and the outer summations $\sum_{\mathbf{h}}$ range over the *hkl* reflections. Choices with low $R_{{\rm merge},i}$ display the chosen symmetry, whereas for those with high $R_{{\rm merge},i}$ the symmetry is inappropriate. The Laue group of highest symmetry with a low $R_{{\rm merge},i}$ is considered the best indication of the Laue group. Several variants of the above procedure exist in the available software. Whichever of them is used, it is important for the discrimination of the averaging process to choose a strategy of data collection such that the intensities of the greatest possible number of Bragg reflections are measured. In practice, validation of symmetry can often be carried out with a few initial images and the data-collection strategy may be based on this assignment.

In the third stage, the intensities of the Bragg reflections are studied to identify the conditions for systematic absences. Some space groups give rise to zero intensity for certain classes of reflections. These 'zeros' occur in a systematic manner and are commonly called systematic absences (*e.g.* in the *h*0*l* class of reflections, if all rows with *l* odd are absent, then the corresponding reflection condition is *h*0*l*: $l = 2n$). In practice, as implemented in software, statistics are produced on the intensity observations of all possible sets of 'reflections conditions' as given in Chapter 2.3 (*e.g.* in the example above, *h*0*l* reflections are separated into sets with $l = 2n$ and those with $l = 2n + 1$). In one approach, the number of observations in each set having an intensity (I) greater than n standard uncertainties [$u(I)$] [*i.e.* $I/u(I) > n$] is displayed for various values of n. Clearly, if a trial condition for systematic absence has observations with strong or medium intensity [*i.e.* $I/u(I) > 3$], the systematic-absence condition is not fulfilled (*i.e.* the reflections are not systematically absent). If there are no such observations, the condition for systematic absence may be valid and the statistics for smaller values of n need then to be examined. These are more problematic to evaluate, as the set of reflections under examination may have many weak reflections due to structural effects of the crystal or to perturbations of the measurements by other systematic effects. An alternative approach to examining numbers of observations is to compare the mean value, $\langle I/u(I) \rangle$, taken over reflections obeying or not a trial reflection condition. For a valid reflection condition, one expects the former value to be considerably larger than the latter. In Section 3.1 of Palatinus & van der Lee (2008), real examples of marginal cases are described.

[3] The tables in Appendix 1.4.4 mentioned above actually deal with space groups in reciprocal space; however, the left part of any entry is just the indices of a reflection generated by the point-group operation corresponding to this entry.

Table 1.6.2.1
The ability of the procedures described in Sections 1.6.2.1 and 1.6.5.1 to distinguish between space groups

The columns of the table show the number of sets of space groups that are indistinguishable by the chosen technique, according to the number of space groups in the set, *e.g.* for Laue-class discrimination, 85 space groups may be uniquely identified, whereas there are 8 sets containing 5 space groups indistinguishable by this technique. The tables in Section 1.6.4 contain 416 different settings of space groups generated from the 230 space-group types.

	No. of space groups in set that are indistinguishable by procedure used					
	1	2	3	4	5	6
No. of sets for Laue-class discrimination	85	78	43	0	8	1
No. of sets for point-group discrimination	390	13	0	0	0	0

The third stage continues by noting that the systematic absences are characteristic of the space group of the crystal, although some sets of space groups have identical reflection conditions. In Chapter 2.3 one finds all the reflection conditions listed individually for the 230 space groups. For practical use in space-group determination, tables have been set up that present a list of all those space groups that are characterized by a given set of reflection conditions. The tables for all the Bravais lattices and Laue groups are given in Section 1.6.4 of this chapter. So, once the reflection conditions have been determined, all compatible space groups can be identified from the tables. Table 1.6.2.1 shows that 85 space groups may be unequivocally determined by the procedures defined in this section based on the identification of the Laue group. For other sets of reflection conditions, there are a larger number of compatible space groups, attaining the value of 6 in one case. It is appropriate at this point to anticipate the results presented in Section 1.6.5.1, which exploit the resonant-scattering contribution to the diffracted intensities and under appropriate conditions allow not only the Laue group but also the point group of the crystal to be identified. If such is the case, the last line of Table 1.6.2.1 shows that almost all space groups can be unequivocally determined. In the remaining 13 pairs of space groups, constituting 26 space groups in all, there are the 11 enantiomorphic pairs of space groups [($P4_1$–$P4_3$), ($P4_122$–$P4_322$), ($P4_12_12$–$P4_32_12$), ($P3_1$–$P3_2$), ($P3_121$–$P3_221$), ($P3_112$–$P3_212$), ($P6_1$–$P6_5$), ($P6_2$–$P6_4$), ($P6_122$–$P6_522$), ($P6_222$–$P6_422$) and ($P4_132$–$P4_332$)] and the two exceptional pairs of $I222$ & $I2_12_12_1$ and $I23$ & $I2_13$, characterized by having the same symmetry elements in a different arrangement in space. These 13 pairs of space groups cannot be distinguished by the methods described in Sections 1.6.2 and 1.6.5.1, but may be distinguished when a reliable atomic structural model of the crystal has been obtained. On the other hand, all these 13 pairs of space groups can be distinguished by the methods described in Section 1.6.6 and in detail in Saitoh *et al.* (2001). It should be pointed out in connection with this third stage that a possible weakness of the analysis of systematic absences for crystals with small unit-cell dimensions is that there may be a small number of axial reflections capable of being systematically absent.

It goes without saying that the selected space groups must be compatible with the Bravais lattice determined in stage 1, with the Laue class determined in stage 2 and with the set of space-group absences determined in stage 3.

We thank L. Palatinus (2011) for having drawn our attention to the unexploited potential of the Patterson function for the determination of the space group of the crystal. The discovery of

this method is due to Buerger (1946) and later obtained only a one-sentence reference by Rogers (1950) and by Rossmann & Arnold (2001). The method is based on the observation that interatomic vectors between symmetry-related (other than by inversion in a point) atoms cause peaks to accumulate in the corresponding Harker sections and lines of the Patterson function. It is thus only necessary to find the location of those Harker sections and lines that have a high concentration of peaks to identify the corresponding symmetry operations of the space group. At the time of its discovery, it was not considered an economic method of space-group determination due to the labour involved in calculating the Patterson function. Subsequently it was completely neglected and there are no recent reports of its use. It is thus not possible to report on its strengths and weaknesses in practical modern-day applications.

1.6.2.2. Structure-factor statistics and crystal symmetry

Most structure-solving software packages contain a section dedicated to several probabilistic methods based on the Wilson (1949) paper on the probability distribution of structure-factor magnitudes. These statistics sometimes correctly indicate whether the intensity data set was collected from a centrosymmetric or noncentrosymmetric crystal. However, not infrequently these indications are erroneous. The reasons for this may be many, but outstandingly important are (i) the presence of a few very heavy atoms amongst a host of lighter ones, and (ii) a very small number of nearly equal atoms. Omission of weak reflections from the data set also contributes to failures of Wilson (1949) statistics. These erroneous indications are also rather strongly space-group dependent.

The well known probability density functions (hereafter p.d.f.'s) of the magnitude of the normalized structure factor E, also known as ideal p.d.f.'s, are

$$p(|E|) = \begin{cases} \sqrt{2/\pi}\exp\left(-|E|^2/2\right) & \text{for } P\overline{1} \\ 2|E|\exp(-|E|^2) & \text{for } P1 \end{cases}, \qquad (1.6.2.3)$$

where it is assumed that all the atoms are of the same chemical element. Let us see their graphical representations.

It is seen from Fig. 1.6.2.1 that the two p.d.f.'s are significantly different, but usually they are not presented as such by the software. What is usually shown are the cumulative distributions of $|E|^2$, the moments: $\langle|E|^n\rangle$ for $n = 1, 2, 3, 4, 5, 6$, and the averages of low powers of $|E^2 - 1|$ for ideal centric and acentric distributions, based on equation (1.6.2.3). Table 1.6.2.2 shows the numerical values of several low-order moments of $|E|$ and that of the lowest power of $|E^2 - 1|$. The higher the value of n the greater is the difference between their values for centric and acentric cases. However, it is most important to remember that the influence of measurement uncertainties also increases with n and therefore the higher the moment the less reliable it tends to be.

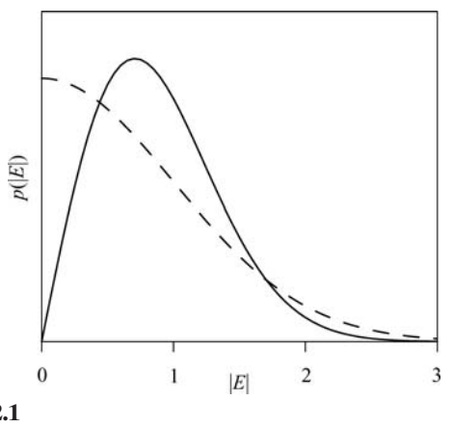

Figure 1.6.2.1
Ideal p.d.f.'s for the equal-atom case. The dashed line is the centric, and the solid line the acentric ideal p.d.f.

Table 1.6.2.2
The numerical values of several low-order moments of $|E|$, based on equation (1.6.2.3)

Moment	$P\overline{1}$	$P1$
$\langle\|E\|\rangle$	0.798	0.886
$\langle\|E\|^2\rangle$	1.000	1.000
$\langle\|E\|^3\rangle$	1.596	1.329
$\langle\|E\|^4\rangle$	3.000	2.000
$\langle\|E\|^5\rangle$	6.383	3.323
$\langle\|E\|^6\rangle$	15.000	6.000
$\langle\|E^2 - 1\|\rangle$	0.968	0.736

There are several ideal indicators of the status of centrosymmetry of a crystal structure. The most frequently used are: (i) the $N(z)$ test (Howells *et al.*, 1950), a cumulative distribution of $z = |E|^2$, based on equation (1.6.2.3), and (ii) the low-order moments of $|E|$, also based on equation (1.6.2.3). Equation (1.6.2.3), however, is very seldom used as an indicator of the status of centrosymmetry of a crystal stucture.

Let us now briefly consider p.d.f.'s that are valid for any atomic composition as well as any space-group symmetry, and exemplify their performance by comparing a histogram derived from observed intensities from a $P\overline{1}$ structure with theoretical p.d.f.'s for the space groups $P1$ and $P\overline{1}$. The p.d.f.'s considered presume that all the atoms are in general positions and that the reflections considered are general (see, *e.g.*, Section 1.6.3). A general treatment of the problem is given in the literature and summarized in the book *Introduction to Crystallographic Statistics* (Shmueli & Weiss, 1995).

The basics of the exact p.d.f.'s are conveniently illustrated in the following. The normalized structure factor for the space group $P\overline{1}$, assuming that all the atoms occupy general positions and resonant scattering is neglected, is given by

$$E(\mathbf{h}) = 2\sum_{j=1}^{N/2} n_j \cos(2\pi\mathbf{h}\boldsymbol{r}_j),$$

where n_j is the normalized scattering factor. The maximum possible value of E is $E_{\max} = \sum_{j=1}^{N} n_j$ and the minimum possible value of E is $-E_{\max}$. Therefore, $E(\mathbf{h})$ must be confined to the $(-E_{\max}, E_{\max})$ range. The probability of finding E outside this range is of course zero. Such a probability density function can be expanded in a Fourier series within this range (*cf.* Shmueli *et al.*, 1984). This is the basis of the derivation, the details of which are well documented (*e.g.* Shmueli *et al.*, 1984; Shmueli & Weiss, 1995; Shmueli, 2007). Exact p.d.f.'s for any centrosymmetric space group have the form

$$p(|E|) = \alpha\left\{1 + 2\sum_{m=1}^{\infty} C_m \cos(\pi m|E|\alpha)\right\}, \qquad (1.6.2.4)$$

where $\alpha = 1/E_{\max}$, and exact p.d.f.'s for any noncentrosymmetric space group can be computed as the double Fourier series

$$p(|E|) = \tfrac{1}{2}\pi\alpha^2|E|\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} C_{mn} J_0[\pi\alpha|E|(m^2 + n^2)^{1/2}], \qquad (1.6.2.5)$$

where $J_0(X)$ is a Bessel function of the first kind and of order zero. Expressions for the coefficients C_m and C_{mn} are given by

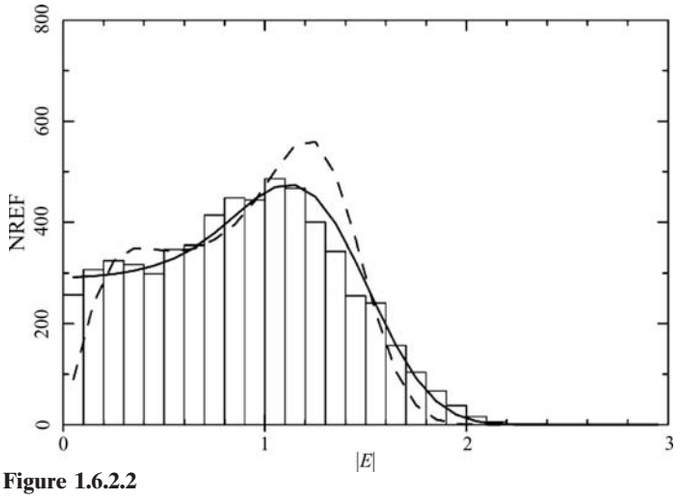

Figure 1.6.2.2
Exact p.d.f.'s. for a crystal of [(*Z*)-ethyl *N*-isopropylthiocarbamato-κS](tricyclohexylphosphine-κP)gold(I) in the triclinic system. Solid curve: $P\overline{1}$, computed from (1.6.2.4); dashed curve: *P*1, computed from (1.6.2.5); histogram based on the data computed from all the reflections with non-negative reduced intensities. The height of each bin corresponds to the number of reflections (NREF) in its range of $|E|$ values. The p.d.f.'s are scaled up to the histogram.

Rabinovich *et al.* (1991) and by Shmueli & Wilson (2008) for all the space groups up to and including $Fd\overline{3}$.

The following example deals with a very high sensitivity to atomic heterogeneity. Consider the crystal structure of [(*Z*)-ethyl *N*-isopropylthiocarbamato-κS](tricyclohexylphosphine-κP)gold(I), published as $P\overline{1}$ with $Z = 2$, the content of its asymmetric unit being $AuSPONC_{24}H_{45}$ (Tadbuppa & Tiekink, 2010). Let us construct a histogram from the $|E|$ data computed from all the observed reflections with non-negative reduced intensities and compare the histogram with the p.d.f.'s for the space groups *P*1 and $P\overline{1}$, computed from equations (1.6.2.5) and (1.6.2.4), respectively. The histogram and the p.d.f.'s were put on the same scale. The result is shown in Fig. 1.6.2.2.

A visual comparison strongly indicates that the space-group assignment as $P\overline{1}$ was correct, since the recalculated histogram agrees rather well with the p.d.f. (1.6.2.4) and much less with (1.6.2.5). The ideal Wilson-type statistics incorrectly indicated that this crystal is noncentrosymmetric. It is seen that the ideal p.d.f. breaks down in the presence of strong atomic heterogeneity (gold among many lighter atoms) in the space group $P\overline{1}$. Other space groups behave differently, as shown in the literature (*e.g.* Rabinovich *et al.*, 1991; Shmueli & Weiss, 1995).

Additional examples of applications of structure-factor statistics and some relevant computing considerations and software can be found in Shmueli (2012) and Shmueli (2013).

1.6.2.3. Symmetry information from the structure solution

It is also possible to obtain information on the symmetry of the crystal after structure solution. The latter is obtained either in space group *P*1 (*i.e.* no symmetry assumed) or in some other candidate space group. The analysis may take place either on the electron-density map, or on its interpretation in terms of atomic coordinates and atomic types (*i.e.* chemical elements). The analysis of the electron-density map has become increasingly popular with the advent of dual-space methods, first proposed in the charge-flipping algorithm by Oszlányi & Sütő (2004), which solve structures in *P*1 by default. The analysis of the atomic coordinates and atomic types obtained from least-squares refinement in a candidate space group is used extensively in structure validation. Symmetry operations present in the structure solution but not in the candidate space group are sought.

An exhaustive search for symmetry operations is undertaken. However, those to be investigated may be very efficently limited by making use of knowledge of the highest point-group symmetry of the lattice compatible with the known cell dimensions of the crystal. It is well established that the point-group symmetry of any lattice is one of the following seven centrosymmetric point groups: $\overline{1}$, 2/*m*, *mmm*, 4/*mmm*, $\overline{3}m$, 6/*mmm*, $m\overline{3}m$. This point group is known as the holohedry of the lattice. The relationship between the symmetry operations of the space group and its holohedry is rather simple. A rotation or screw axis of symmetry in the crystal has as its counterpart a corresponding rotation axis of symmetry of the lattice and a mirror or glide plane in the crystal has as its counterpart a corresponding mirror plane in the lattice. The holohedry may be equal to or higher than the point group of the crystal. Hence, at least the rotational part of any space-group operation should have its counterpart in the symmetry of the lattice. If and when this rotational part is found by a systematic comparison either of the electron density or of the positions of the independent atoms of the solved structure, the location and intrinsic parts of the translation parts of the space-group operation can be easily completed.

Palatinus and van der Lee (2008) describe their procedure in detail with useful examples. It uses the structure solution both in the form of an electron-density map and a set of phased structure factors obtained by Fourier transformation. No interpretation of the electron-density map in the form of atomic coordinates and chemical-element type is required. The algorithm of the procedure proceeds in the following steps:

(1) The lattice centring is determined by a search for strong peaks in the autocorrelation (self-convolution, Patterson) function of the electron density and the potential centring vectors are evaluated through a reciprocal-space *R* value.
(2) A complete list of possible symmetry operations compatible with the lattice is generated by searching for the invariance of the direct-space metric under potential symmetry operations.
(3) A figure of merit is then assigned to each symmetry operation evaluated from the convolution of the symmetry-transformed electron density with that of the structure solution. Those symmetry operations that have a good figure of merit are selected as belonging to the space group of the crystal structure.
(4) The space group is completed by group multiplication of the selected operations and then validated.
(5) The positions of the symmetry elements are shifted to those of a conventional setting for the space group.

Palatinus & van der Lee (2008) report a very high success rate in the use of this algorithm. It is also a powerful technique to apply in structure validation.

Le Page's (1987) pioneering software *MISSYM* for the detection of 'missed' symmetry operations uses refined atomic coordinates, unit-cell dimensions and space group assigned from the crystal-structure solution. The algorithm follows all the principles described above in this section. In *MISSYM*, the metric symmetry is established as described in the first stage of Section 1.6.2.1. The 'missed' symmetry operations are those that are present in the arrangement of the atoms but are not part of the space group used for the structure refinement. Indeed, this procedure has its main applications in structure validation. The algorithm used in Le Page's software is also implemented in *ADDSYM* (Spek, 2003). There are numerous reports of successful applications of this software in the literature.

1.6.2.4. Restrictions on space groups

The values of certain chemical and physical properties of a bulk compound, or its crystals, have implications for the assignment of the space group of a crystal structure. In the chemical domain, notably in proteins and small-molecule natural products, information concerning the enantiomeric purity of the bulk compound or of its individual crystals is most useful. Further, all physical properties of a crystal are limited by the point group of the crystal structure in ways that depend on the individual nature of the physical property.

It is very well established that the crystal structure of an enantiomerically pure compound will be chiral (see Flack, 2003). By an enantiomerically pure compound one means a compound whose molecules are all chiral and all these molecules possess the same chirality. The space group of a chiral crystal structure will only contain the following types of symmetry operation: translations, pure rotations and screw rotations. Inversion in a point, mirror reflection or rotoinversion do not occur in the space group of a chiral crystal structure. Taking all this together means that the crystal structure of an enantiomerically pure compound will show one of 65 space groups (known as the Sohncke space groups), all noncentrosymmetric, containing only translations, rotations and screw rotations. As a consequence, the point group of a chiral crystal structure is limited to the 11 point groups containing only pure rotations (*i.e.* 1, 2, 222, 4, 422, 3, 32, 6, 622, 23 and 432). Particular attention must be paid as to whether a measurement of enantiomeric purity of a compound applies to the bulk material or to the single crystal used for the diffraction experiment. Clearly, a compound whose bulk is enantiomerically pure will produce crystals which are enantiomerically pure. The converse is not necessarily true (*i.e.* enantiomerically pure crystals do not necessarily come from an enantiomerically pure bulk). For example, a bulk compound which is a racemate (*i.e.* an enantiomeric mixture containing 50% each of the opposite enantiomers) may produce either (*a*) crystals of the racemic compound (*i.e.* crystals containing 50% each of the opposite enantiomers) or (*b*) a racemic conglomerate (*i.e.* a mixture of enantiomerically pure crystals in a proportion of 50% of each pure enantiomer) or (*c*) some other rarer crystallization modes. Consequently, as part of a single-crystal structure analysis, it is highly recommended to make a measurement of the enantiomeric purity of the single crystal used for the diffraction experiment.

Much information on methods of establishing the enantiomeric purity of a compound can be found in a special issue of *Chirality* devoted to the determination of absolute configuration (Allenmark *et al.*, 2007). Measurements in the fluid state of optical activity, optical rotatory dispersion (ORD), circular dichroism (CD) and enantioselective chromatography are of prime importance. Many of these are sufficiently sensitive to be applicable not only to the bulk compound but also to the single crystal used for the diffraction experiment taken into solution. CD may also be applied in the solid state.

Many physical properties of a crystalline solid are anisotropic and the symmetry of a physical property of a crystal is limited both by the point-group symmetry of the crystal and by symmetries inherent to the physical property under study. For further information on this topic see Part 1 of Volume D (Authier *et al.*, 2014). Unfortunately, many of these physical properties are intrinsically centrosymmetric, so few of them are of use in distinguishing between the subgroups of a Laue group, a common problem in space-group determination. In Chapter 3.2 of the present volume, Hahn & Klapper show to which point groups a crystal must belong to be capable of displaying some of the principal physical properties of crystals (Table 3.2.2.1). Measurement of morphology, pyroelectricity, piezoelectricity, second harmonic generation and optical activity of a crystalline sample can be of use.

1.6.2.5. Pitfalls in space-group determination

The methods described in Sections 1.6.2 and 1.6.5.1 rely on the crystal measured being a single-domain crystal, *i.e.* it should not be twinned. Nevertheless, some types of twin are easily identified at the measurement stage as they give rise to split reflections. Powerful data-reduction techniques may be applied to data from such crystals to produce a reasonably complete single-domain intensity data set. Consequently, the multi-domain twinned crystals that give rise to difficulties in space-group determination are those for which the reciprocal lattices of the individual domains overlap exactly without generating any splitting of the Bragg reflections. A study of the intensity data from such a crystal may display two anomalies. Firstly, the intensity distribution, as described and analysed in Section 1.6.2.2, will be broader than that of the monodomain crystal. Secondly, one may obtain a set of conditions for reflections that does not correspond to any entry in Section 1.6.4. In this chapter we give no further information on the determination of the space group for such twinned crystals. For further information on this topic see Part 3 of Volume D (Boček *et al.*, 2006) and Chapter 1.3 on twinning in Volume C (Koch, 2006). A supplement (Flack, 2015) to the current section deals with the determination of the space group from twinned crystals and those displaying a specialized metric. However, it is apposite to note that the existence of twins with overlapping reciprocal lattices can be identified by recording atomic resolution transmission electron-microscope images.

In order to obtain reliable results from space-group determination, the coverage of the reciprocal space by the intensity measurements should be as complete as possible. One should attempt to attain full-sphere data coverage, *i.e.* a complete set of intensity measurements in the point group 1. All Friedel opposites should be measured. The validity and reliability of the intensity statistics described in Section 1.6.2.2 rest on a full coverage of reciprocal lattice. Any systematic omission by resolution, azimuth and declination, intensity *etc.* of part of the asymmetric region of the reciprocal lattice has an adverse effect. In particular, reflections of weak intensity should not be omitted or deleted.

There are a few other common difficulties in space-group determination due either to the nature of the crystal or the experimental setup:

(*a*) The crystal may display a pseudo-periodicity leading to systematic series of weak or very weak reflections that can be mistaken for systematic absences.

(*b*) The physical effect of multiple reflections can lead to diffraction intensity appearing at the place of systematic absences. However, the shape of these multiple-reflection intensities is usually much sharper than a normal Bragg reflection.

(*c*) Contamination of the incident radiation by a $\lambda/2$ component may also cause intensity due to the $2h\,2k\,2l$ reflection to appear at the place of the hkl one. Kirschbaum *et al.* (1997) and Macchi *et al.* (1998) have studied this probem and describe ways of circumventing it.

1.6.3. Theoretical background of reflection conditions

By U. Shmueli

We shall now examine the effect of the space-group symmetry on the structure-factor function. These effects are of importance in the determination of crystal symmetry. If $(\boldsymbol{W}, \boldsymbol{w})$ is the matrix–column pair of a representative symmetry operation of the space group of the crystal, then, by definition

$$\rho(\boldsymbol{x}) = \rho(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}), \tag{1.6.3.1}$$

where $\rho(\boldsymbol{x})$ is the value of the electron-density function at the point with coordinates $\boldsymbol{x}$, $\boldsymbol{W}$ is a matrix of proper or improper rotation and $\boldsymbol{w}$ is a translation part (*cf.* Section 1.2.2.1). It is known that the electron-density function at the point $\boldsymbol{x}$ is given by

$$\rho(\boldsymbol{x}) = \frac{1}{V}\sum_{\mathbf{h}} F(\mathbf{h}) \exp(-2\pi i \mathbf{h}\boldsymbol{x}), \tag{1.6.3.2}$$

where, in this and the following equations, $\mathbf{h}$ is the row matrix $(h\,k\,l)$ and $\boldsymbol{x}$ is a column matrix containing x, y and z in the first, second and third rows, respectively. Of course, $\mathbf{h}\boldsymbol{x}$ is simply equivalent to $hx + ky + lz$. If we substitute (1.6.3.2), with $\boldsymbol{x}$ replaced by $(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{w})$ in (1.6.3.1) we obtain, after some calculation,

$$F(\mathbf{h}\boldsymbol{W}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}\boldsymbol{w}). \tag{1.6.3.3}$$

Equation (1.6.3.3) is the fundamental relation between symmetry-related reflections (*e.g.* Waser, 1955; Wells, 1965; and Chapter 1.4 in Volume B). If we write $F(\mathbf{h}) = |F(\mathbf{h})| \exp[i\varphi(\mathbf{h})]$, equation (1.6.3.3) leads to the following relationships:

$$|F(\mathbf{h}\boldsymbol{W})| = |F(\mathbf{h})| \tag{1.6.3.4}$$

and

$$\varphi(\mathbf{h}\boldsymbol{W}) = \varphi(\mathbf{h}) - 2\pi\mathbf{h}\boldsymbol{w}. \tag{1.6.3.5}$$

Equation (1.6.3.4) indicates the equality of the intensities of truly symmetry-related reflections, while equation (1.6.3.5) relates the phases of the corresponding structure factors. The latter equation is of major importance in direct methods of phase determination [*e.g.* Chapter 2.2 in Volume B (Giacovazzo, 2008)].

We can now approach the problem of systematically absent reflections, which are alternatively called the conditions for possible reflections.

The reflection $\mathbf{h}$ is *general* if its indices remain unchanged *only* under the identity operation of the point group of the diffraction pattern. *I.e.*, if $\boldsymbol{W}$ is the matrix of the identity operation of the point group, the relation $\mathbf{h}\boldsymbol{W} = \mathbf{h}$ holds true. So, if the reflection $\mathbf{h}$ is general, we must have $\boldsymbol{W} \equiv \boldsymbol{I}$, where $\boldsymbol{I}$ is the identity matrix and, obviously, $\mathbf{h}\boldsymbol{I} = \mathbf{h}$. The operation $(\boldsymbol{I}, \boldsymbol{w})$ can be a space-group symmetry operation only if $\boldsymbol{w}$ is a lattice vector. Let us denote it by $\boldsymbol{w}_L$. Equation (1.6.3.3) then reduces to

$$F(\mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}\boldsymbol{w}_L) \tag{1.6.3.6}$$

and $F(\mathbf{h})$ can be nonzero only if $\exp(-2\pi i \mathbf{h}\boldsymbol{w}_L) = 1$. This, in turn, is possible only if $\mathbf{h}\boldsymbol{w}_L$ is an integer and leads to conditions depending on the lattice type. For example, if the components of $\boldsymbol{w}_L$ are all integers, which is the case for a *P*-type lattice, the above condition is fulfilled for all $\mathbf{h}$ – the lattice type does not impose any restrictions. If the lattice is of type *I*, there are two lattice points in the unit cell, at say 0, 0, 0 and 1/2, 1/2, 1/2. The first of these does not lead to any restrictions on possible reflections. The second, however, requires that $\exp[-\pi i(h + k + l)]$ be equal to unity. Since $\exp(\pi i n) = (-1)^n$, where n is an integer, the possible reflections from a crystal with an *I*-type lattice must have indices such that their sum is an even integer; if the sum of the indices is an odd integer, the reflection is *systematically absent*. In this way, we examine all lattice types for conditions of possible reflections (or systematic absences) and present the results in Table 1.6.3.1.

The reflection $\mathbf{h}$ is *special* if it remains unchanged under at least one operation of the point group of the diffraction pattern in addition to its identity operation. *I.e.*, the relation $\mathbf{h}\boldsymbol{W} = \mathbf{h}$ holds true for more than one operation of the point group. We shall now assume that the reflection $\mathbf{h}$ is special. By definition, this reflection remains invariant under more than one operation of the point group of the diffraction pattern. These operations form a subgroup of the point group of the diffraction pattern, known as the stabilizer (formerly called the *isotropy subgroup*) of the reflection $\mathbf{h}$, and we denote it by the symbol $\mathcal{S}_{\mathbf{h}}$. For each space-group symmetry operation $(\boldsymbol{W}, \boldsymbol{w})$ where $\boldsymbol{W}$ is the matrix of an element of $\mathcal{S}_{\mathbf{h}}$ we must therefore have $\mathbf{h}\boldsymbol{W} = \mathbf{h}$. Equation (1.6.3.3) now reduces to

$$F(\mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}\boldsymbol{w}). \tag{1.6.3.7}$$

Of course, if $\boldsymbol{W}$ represents the identity operation, $\boldsymbol{w}$ must be a lattice vector and the discussion summarized in Table 1.6.3.1 applies. We therefore require that $\boldsymbol{W}$ is the matrix of an element of $\mathcal{S}_{\mathbf{h}}$ other than the identity. $F(\mathbf{h})$ can be nonzero only if the exponential factor in (1.6.3.7) equals unity. This, in turn, is possible only if $\mathbf{h}\boldsymbol{w}$ is an integer.

Let us consider a monoclinic crystal with *P*-type lattice (*i.e.* with an *mP*-type Bravais lattice) and a *c*-glide reflection as an example. Assuming $\mathbf{b}$ perpendicular to the $\mathbf{ac}$ plane, the $(\boldsymbol{W}, \boldsymbol{w})$ representation of *c* is given by

$$c\colon \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & \overline{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ y \\ 1/2 \end{pmatrix}\right].$$

The indices of reflections that remain unchanged under the application of the mirror component of the glide-reflection operation must be $h0l$. The translation part of the *c*-glide-reflection operation has the form $(0, y, 1/2)$, where $y = 0$ corresponds to the plane passing through the origin. Hence, for any value of y, the scalar product $\mathbf{h}\boldsymbol{w}$ is $l/2$ and the necessary condition for a nonzero value of an $h0l$ reflection is $l = 2n$, where n is an integer. Intensities of $h0l$ reflections with odd l will be *systematically absent*.

Table 1.6.3.2 shows the effect of some glide reflections on reflection conditions.[4]

Let us now assume a crystal with an *mP*-type Bravais lattice and a twofold screw axis taken as being parallel to $\mathbf{b}$. The $(\boldsymbol{W}, \boldsymbol{w})$ representation of the corresponding screw rotation is given by

$$2_1\colon \left[\begin{pmatrix} \overline{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \overline{1} \end{pmatrix}, \begin{pmatrix} x \\ 1/2 \\ z \end{pmatrix}\right].$$

The diffraction indices that remain unchanged upon the application of the rotation part of 2_1 must be of the form $(0k0)$. The translation part of the screw operation is of the form $(x, 1/2, z)$, where the values of x and z depend on the location of the origin. Hence, for any values of x and z the scalar product $\mathbf{h}\boldsymbol{w}$ is $k/2$ and the necessary condition for a nonzero value of a $0k0$ reflection is

[4] The reflection condition in the fourth line of Table 1.6.3.2 is a consequence of the fact that a *d* glide appears only with Bravais lattices of types *I* and *F*.

Table 1.6.3.1
Effect of lattice type on conditions for possible reflections

Lattice type	$\boldsymbol{w}_L^T$	$\mathbf{h}\boldsymbol{w}_L$	Conditions for possible reflections
P	(0, 0, 0)	Integer	None
A	$(0, \frac{1}{2}, \frac{1}{2})$	$(k+l)/2$	hkl: $k+l=2n$
B	$(\frac{1}{2}, 0, \frac{1}{2})$	$(h+l)/2$	hkl: $h+l=2n$
C	$(\frac{1}{2}, \frac{1}{2}, 0)$	$(h+k)/2$	hkl: $h+k=2n$
I	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$(h+k+l)/2$	hkl: $h+k+l=2n$
F	$(0, \frac{1}{2}, \frac{1}{2})$	$(k+l)/2$	h, k and l are all even or all odd (simultaneous fulfillment of the conditions for types A, B and C).
	$(\frac{1}{2}, 0, \frac{1}{2})$	$(h+l)/2$	
	$(\frac{1}{2}, \frac{1}{2}, 0)$	$(h+k)/2$	
$R_{\rm obv}$	$(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$	$(2h+k+l)/3$	hkl: $-h+k+l=3n$
	$(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$	$(h+2k+2l)/3$	(triple hexagonal cell in obverse orientation)
$R_{\rm rev}$	$(\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$	$(h+2k+l)/3$	hkl: $h-k+l=3n$
	$(\frac{2}{3}, \frac{1}{3}, \frac{2}{3})$	$(2h+k+2l)/3$	(triple hexagonal cell in reverse orientation)

Table 1.6.3.2
Effect of some glide reflections on conditions for possible reflections

Glide reflection	$\boldsymbol{w}^T$	$\mathbf{h}$	Conditions for possible reflections
$a \perp [001]$	(1/2, 0, z)	(hk0)	hk0: $h=2n$
$b \perp [001]$	(0, 1/2, z)	(hk0)	hk0: $k=2n$
$n \perp [001]$	(1/2, 1/2, z)	(hk0)	hk0: $h+k=2n$
$d \perp [001]$	(1/4, $\pm$1/4, z)	(hk0)	hk0: $h+k=4n$ (h, $k=2n$)

Table 1.6.3.3
Effect of some screw rotations on conditions for possible reflections

Screw rotation	$\boldsymbol{w}^T$	$\mathbf{h}$	Conditions for possible reflections
$2_1 \parallel [100]$	(1/2, y, z)	(h00)	h00: $h=2n$
$2_1 \parallel [010]$	(x, 1/2, z)	(0k0)	0k0: $k=2n$
$2_1 \parallel [001]$	(x, y, 1/2)	(00l)	00l: $l=2n$
$2_1 \parallel [110]$	(1/2, 1/2, z)	(hh0)	None
$3_1 \parallel [001]$	(x, y, 1/3)	(00l)	00l: $l=3n$
$3_1 \parallel [111]$	(1/3, 1/3, 1/3)	(hhh)	None
$4_1 \parallel [001]$	(x, y, 1/4)	(00l)	00l: $l=4n$
$6_1 \parallel [001]$	(x, y, 1/6)	(00l)	00l: $l=6n$

$k=2n$. 0k0 reflections with odd k will be systematically absent. A brief summary of the effects of various screw rotations on the conditions for possible reflections from the corresponding special subsets of hkl is given in Table 1.6.3.3. Note, however, that while the presence of a twofold screw axis parallel to **b** ensures the condition 0k0: $k=2n$, the actual observation of such a condition can be taken as an indication but not as absolute proof of the presence of a screw axis in the crystal.

It is interesting to note that some diagonal screw axes do not give rise to conditions for possible reflections. For example, let $\boldsymbol{W}$ be the matrix of a threefold rotation operation parallel to [111] and $\boldsymbol{w}^T$ be given by (1/3, 1/3, 1/3). It is easy to show that the diffraction vector that remains unchanged when postmultiplied by $\boldsymbol{W}$ has the form $\mathbf{h}=(hhh)$ and, obviously, for such **h** and $\boldsymbol{w}$, $\mathbf{h}\boldsymbol{w}=h$. Since this scalar product is an integer there are, according to equation (1.6.3.7), no values of the index h for which the structure factor $F(hhh)$ must be absent.

A short discussion of special reflection conditions

The conditions for possible reflections arising from lattice types, glide reflections and screw rotations are related to general equivalent positions and are known as *general reflection conditions*. There are also *special* or '*extra*' reflection conditions that arise from the presence of atoms in special positions. These conditions are observable if the atoms located in special positions are much heavier than the rest. The minimal special conditions are listed in the space-group tables in Chapter 2.3. They can sometimes be understood if the geometry of a given specific site is examined. For example, Wyckoff position 4i in space group $P4_222$ (93) can host four atoms, at coordinates

$$4i\colon\ 0, \tfrac{1}{2}, z;\ \ \tfrac{1}{2}, 0, z+\tfrac{1}{2};\ \ 0, \tfrac{1}{2}, \overline{z};\ \ \tfrac{1}{2}, 0, \overline{z}+\tfrac{1}{2}.$$

It is seen that the second and fourth coordinates are obtained from the first and third coordinates, respectively, upon the addition of the vector $t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. An additional I-centring is therefore present in this set of special positions. Hence, the special reflection condition for this set is hkl: $h+k+l=2n$.

It should be pointed out, however, that only the general reflection conditions are used for a complete or partial determination of the space group and that the special reflection conditions only apply to spherical atoms. By the latter assumption we understand not only the assumption of spherical distribution of the atomic electron density but also isotropic displacement parameters of the equivalent atoms that belong to the set of corresponding special positions.

One method of finding the minimal special reflection conditions for a given set of special positions is the evaluation of the trigonometric structure factor for the set in question. For example, consider the Wyckoff position 4c of the space group $Pbcm$ (57). The coordinates of the special equivalent positions are

$$4c\colon\ \ x, \tfrac{1}{4}, 0;\quad \overline{x}, \tfrac{3}{4}, \tfrac{1}{2};\quad \overline{x}, \tfrac{3}{4}, 0;\quad x, \tfrac{1}{4}, \tfrac{1}{2}$$

and the corresponding trigonometric structure factor is

$$S(\mathbf{h}) = \exp\left[2\pi i\left(hx+\frac{k}{4}\right)\right] + \exp\left[2\pi i\left(-hx+\frac{3k}{4}+\frac{l}{2}\right)\right] + \exp\left[2\pi i\left(-hx+\frac{3k}{4}\right)\right] + \exp\left[2\pi i\left(hx+\frac{k}{4}+\frac{l}{2}\right)\right].$$

It can be easily shown that

$$S(\mathbf{h}) = 2\cos\left[2\pi\left(hx+\frac{k}{4}\right)\right][1+\exp(\pi i l)]$$

and the last factor equals 2 for l even and equals zero for l odd. The special reflection condition is therefore: hkl: $l=2n$.

Another approach is provided by considerations of the eigensymmetry group and the extraordinary orbits of the space group (see Section 1.4.4.4). We recall that the eigensymmetry group is a group of all the operations that leave the orbit of a point under the space group considered invariant, and the extraordinary orbit is associated with the eigensymmetry group that contains translations not present in the space group (see Chapter 1.4). In the above example the orbit is extraordinary, since its eigensymmetry group contains a translation corresponding to $\frac{1}{2}\mathbf{c}$. If this is taken as a basis vector, we have the Laue equation $\frac{1}{2}\mathbf{c}\cdot\mathbf{h}=l'$, where **h** is represented as a reciprocal-lattice vector and l' is an integer which also equals $l/2$. But for $l/2$ to be an integer we must have even l. We again obtain the condition hkl: $l=2n$.

These reflection conditions that are not related to space-group operations are given in Chapter 2.3 only for special positions. They may arise, however, also for different reasons. For example, a heavy atom at the origin of the space group $P2_12_12_1$ would generate *F*-centring with corresponding apparent absences (*cf.* the special position 4*a* of the space group *Pbca* and the absences it generates).

We wish to point out that the most common 'special-position absence' in molecular structures is due to a heavy atom at the origin of the space group $P2_1/c$.

1.6.4. Tables of reflection conditions and possible space groups

By H. D. Flack and U. Shmueli

1.6.4.1. Introduction

The primary order of presentation of these tables of reflection conditions of space groups is the Bravais lattice. This order has been chosen because cell reduction on unit-cell dimensions leads to the Bravais lattice as described as stage 1 in Section 1.6.2.1. Within the space groups of a given Bravais lattice, the entries are arranged by Laue class, which may be obtained as described as stage 2 in Section 1.6.2.1. As a consequence of these decisions about the way the tables are structured, in the hexagonal family one finds for the Bravais lattice *hP* that the Laue classes $\overline{3}$, $\overline{3}m1$, $\overline{3}1m$, 6/*m* and 6/*mmm* are grouped together.

As an aid in the study of naturally occurring macromolecules and compounds made by enantioselective synthesis, the space groups of enantiomerically pure compounds (Sohncke space groups) are typeset in bold.

The tables show, on the left, sets of reflection conditions and, on the right, those space groups that are compatible with the given set of reflection conditions. The reflection conditions, *e.g.* *h* or $k + l$, are to be understood as $h = 2n$ or $k + l = 2n$, respectively. All of the space groups in each table correspond to the same Patterson symmetry, which is indicated in the table header. This makes for easy comparison with the entries for the individual space groups in Chapter 2.3 of this volume, in which the Patterson symmetry is also very clearly shown. All space groups with a conventional choice of unit cell are included in Tables 1.6.4.2–1.6.4.30. All alternative settings displayed in Chapter 2.3 are thus included. The following further alternative settings, not displayed in Chapter 2.3, are also included: space group $Pb\overline{3}$ (205) and all the space groups with an *hR* Bravais lattice in the reverse setting with hexagonal axes.

Table 1.6.2.1 gives some relevant statistics drawn from Tables 1.6.4.2–1.6.4.30. The total number of space-group settings mentioned in these tables is 416. This number is considerably larger than the 230 space-group types described in Part 2 of this volume. The following example shows why the tables include data for several descriptions of the space-group types. At the stage of space-group determination for a crystal in the crystal class *mm*2, it is not yet known whether the twofold rotation axis lies along **a**, **b** or **c**. Consequently, space groups based on the three point groups 2*mm,* *m*2*m* and *mm*2 need to be considered.

In some texts dealing with space-group determination, a 'diffraction symbol' (sometimes also called an 'extinction symbol') in the form of a Hermann–Mauguin space-group symbol is used as a shorthand code for the reflection conditions and Laue class. These symbols were introduced by Buerger (1935, 1942, 1969) and a concise description is to be found in Looijenga-Vos & Buerger (2002). Nespolo *et al.* (2014) use them.

1.6.4.2. Examples of the use of the tables

(1) If the Bravais lattice is *oI* and the Laue class is *mmm*, Table 1.6.4.1 directs us to Table 1.6.4.11. Given the observed reflection conditions

$$hkl\colon h + k + l = 2n, \quad 0kl\colon k = 2n, l = 2n, \quad h0l\colon h + l = 2n,$$
$$hk0\colon h + k = 2n, \quad h00\colon h = 2n, \quad 0k0\colon k = 2n, \quad 00l\colon l = 2n,$$

it is seen from Table 1.6.4.11 that the possible settings of the space groups are: *Ibm*2 (46), *Ic*2*m* (46), *Ibmm* (74) and *Icmm* (74).

(2) If the Bravais lattice is *oP* and the Laue class is *mmm*, Table 1.6.4.1 directs us to Table 1.6.4.7. If there are no conditions on 0*kl*, the space groups *P*222 to *Pmnn* should be searched. If the condition is 0*kl*: $k = 2n$ or $l = 2n$, the space groups *Pbm*2 to *Pcnn* should be searched. If the condition is 0*kl*: $k + l = 2n$, the space groups $Pnm2_1$ to *Pnnn* should be searched.

(3) If the Bravais lattice is *cP* and the Laue class is $m\overline{3}$, Table 1.6.4.1 directs us to Table 1.6.4.25. If the conditions are 0*kl*: $k = 2n$ and *h*00: $h = 2n$, it is readily seen that the space group is $Pa\overline{3}$.

(4) If only the Bravais lattice is known or assumed, which is the case in powder-diffraction work (see Section 1.6.5.3), all tables of this section corresponding to this Bravais lattice need to be consulted. For example, if it is known that the Bravais lattice is of type *cP*, Table 1.6.4.1 tells us that the possible Laue classes are $m\overline{3}$ and $m\overline{3}m$, and the possible space groups can be found in Tables 1.6.4.25 and 1.6.4.26, respectively. The appropriate reflection conditions are of course given in these tables. All relevant tables can thus be located with the aid of Table 1.6.4.1 if the Bravais lattice is known.

1.6.5. Specialized methods of space-group determination

By H. D. Flack

1.6.5.1. Applications of resonant scattering to symmetry determination

1.6.5.1.1. Introduction

In small-molecule crystallography, it has been customary in crystal-structure analysis to make no use of the contribution of resonant scattering (otherwise called anomalous scattering and in older literature anomalous dispersion) other than in the specific area of absolute-structure and absolute-configuration determination. One may trace the causes of this situation to the weakness of the resonant-scattering contribution, to the high cost in time and labour of collecting intensity data sets containing measurements of all Friedel opposites and for a lack of any perceived or real need for the additional information that might be obtained from the effects of resonant scattering.

On the experimental side, the turning point came with the widespread distribution of area detectors for small-molecule crystallography, giving the potential to measure, at no extra cost, full-sphere data sets leading to the intensity differences between Friedel opposites *hkl* and $\overline{hkl}$. In 2015, the new methods of data analysis briefly presented here are in the stage of development

(*continued on page* 125)

Table 1.6.4.1
Summary of Tables 1.6.4.2–1.6.4.30

Table No.	Bravais lattice	Laue class	Patterson symmetry	Comment
1.6.4.2	*aP*	$\bar{1}$	$P\bar{1}$	
1.6.4.3	*mP*	2/*m*	*P*12/*m*1	Unique *b*
1.6.4.4	*mS* (*mC*, *mA*, *mI*)	2/*m*	*C*12/*m*1, *A*12/*m*1, *I*12/*m*1	Unique *b*
1.6.4.5	*mP*	2/*m*	*P*112/*m*	Unique *c*
1.6.4.6	*mS* (*mA*, *mB*, *mI*)	2/*m*	*A*112/*m*, *B*112/*m*, *I*112/*m*	Unique *c*
1.6.4.7	*oP*	*mmm*	*Pmmm*	
1.6.4.8	*oS* (*oC*)	*mmm*	*Cmmm*	
1.6.4.9	*oS* (*oB*)	*mmm*	*Bmmm*	
1.6.4.10	*oS* (*oA*)	*mmm*	*Ammm*	
1.6.4.11	*oI*	*mmm*	*Immm*	
1.6.4.12	*oF*	*mmm*	*Fmmm*	
1.6.4.13	*tP*	4/*m*	*P*4/*m*	
1.6.4.14	*tP*	4/*mmm*	*P*4/*mmm*	
1.6.4.15	*tI*	4/*m*	*I*4/*m*	
1.6.4.16	*tI*	4/*mmm*	*I*4/*mmm*	
1.6.4.17	*hP*	$\bar{3}$	$P\bar{3}$	
1.6.4.18	*hP*	$\bar{3}1m$ and $\bar{3}m1$	$P\bar{3}1m$ and $P\bar{3}m1$	
1.6.4.19	*hP*	6/*m*	*P*6/*m*	
1.6.4.20	*hP*	6/*mmm*	*P*6/*mmm*	
1.6.4.21	*hR*	$\bar{3}$	$R\bar{3}$	Hexagonal axes
1.6.4.22	*hR*	$\bar{3}m$	$R\bar{3}m$	Hexagonal axes
1.6.4.23	*hR*	$\bar{3}$	$R\bar{3}$	Rhombohedral axes
1.6.4.24	*hR*	$\bar{3}m$	$R\bar{3}m$	Rhombohedral axes
1.6.4.25	*cP*	$m\bar{3}$	$Pm\bar{3}$	
1.6.4.26	*cP*	$m\bar{3}m$	$Pm\bar{3}m$	
1.6.4.27	*cI*	$m\bar{3}$	$Im\bar{3}$	
1.6.4.28	*cI*	$m\bar{3}m$	$Im\bar{3}m$	
1.6.4.29	*cF*	$m\bar{3}$	$Fm\bar{3}$	
1.6.4.30	*cF*	$m\bar{3}m$	$Fm\bar{3}m$	

Table 1.6.4.2
Reflection conditions and possible space groups with Bravais lattice *aP* and Laue class $\bar{1}$; Patterson symmetry $P\bar{1}$

Reflection conditions	Space group	No.	Space group	No.
	***P*1**	1	$P\bar{1}$	2

Table 1.6.4.3
Reflection conditions and possible space groups with Bravais lattice *mP* and Laue class 2/*m*; (monoclinic, unique axis *b*); Patterson symmetry *P*12/*m*1

Reflection conditions						Space group	No.	Space group	No.	Space group	No.
*h*0*l*	0*kl*	*hk*0	0*k*0	*h*00	00*l*						
						***P*2**	3	*Pm*	6	*P*2/*m*	10
			k			***P*2$_1$**	4	*P*2$_1$/*m*	11		
h				*h*		*Pa*	7	*P*2/*a*	13		
h			*k*	*h*		*P*2$_1$/*a*	14				
l					*l*	*Pc*	7	*P*2/*c*	13		
l			*k*		*l*	*P*2$_1$/*c*	14				
h + *l*				*h*	*l*	*Pn*	7	*P*2/*n*	13		
h + *l*			*k*	*h*	*l*	*P*2$_1$/*n*	14				

Table 1.6.4.4
Reflection conditions and possible space groups with Bravais lattice *mS* (*mC*, *mA*, *mI*) and Laue class 2/*m* (monoclinic, unique axis *b*); Patterson symmetry *C*12/*m*1, *A*12/*m*1, *I*12/*m*1

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	*h*0*l*	0*kl*	*hk*0	0*k*0	*h*00	00*l*						
$h + k$	h	k	$h + k$	k	h		***C*2**	5	*Cm*	8	*C*2/*m*	12
$h + k$	h, l	k	$h + k$	k	h	l	*Cc*	9	*C*2/*c*	15		
$k + l$	l	$k + l$	k	k		l	***A*2**	5	*Am*	8	*A*2/*m*	12
$k + l$	h, l	$k + l$	k	k	h	l	*An*	9	*A*2/*n*	15		
$h + k + l$	$h + l$	$k + l$	$h + k$	k	h	l	***I*2**	5	*Im*	8	*I*2/*m*	12
$h + k + l$	h, l	$k + l$	$h + k$	k	h	l	*Ia*	9	*I*2/*a*	15		

Table 1.6.4.5
Reflection conditions and possible space groups with Bravais lattice *mP* and Laue class 2/*m* (monoclinic, unique axis *c*); Patterson symmetry *P*112/*m*

Reflection conditions						Space group	No.	Space group	No.	Space group	No.
*h*0*l*	0*kl*	*hk*0	0*k*0	*h*00	00*l*						
						***P*2**	3	*Pm*	6	*P*2/*m*	10
					l	***P*2$_1$**	4	*P*2$_1$/*m*	11		
		h		h		*Pa*	7	*P*2/*a*	13		
		h		h	l	*P*2$_1$/*a*	14				
		k	k			*Pb*	7	*P*2/*b*	13		
		k	k		l	*P*2$_1$/*b*	14				
		$h + k$	k	h		*Pn*	7	*P*2/*n*	13		
		$h + k$	k	h	l	*P*2$_1$/*n*	14				

Table 1.6.4.6
Reflection conditions and possible space groups with Bravais lattice *mS* (*mA*, *mB*, *mI*) and Laue class 2/*m* (monoclinic, unique axis *c*); Patterson symmetry *A*112/*m*, *B*112/*m*1, *I*112/*m*

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	*h*0*l*	0*kl*	*hk*0	0*k*0	*h*00	00*l*						
$k + l$	l	$k + l$	k	k		l	***A*2**	5	*Am*	8	*A*2/*m*	12
$k + l$	l	$k + l$	h, k	k	h	l	*Aa*	9	*A*2/*a*	15		
$h + l$	$h + l$	l	h		h	l	***B*2**	5	*Bm*	8	*B*2/*m*	12
$h + l$	$h + l$	l	h, k	k	h	l	*Bn*	9	*B*2/*n*	15		
$h + k + l$	$h + l$	$k + l$	$h + k$	k	h	l	***I*2**	5	*Im*	8	*I*2/*m*	12
$h + k + l$	$h + l$	$k + l$	h, k	k	h	l	*Ib*	9	*I*2/*b*	15		

Table 1.6.4.7
Reflection conditions and possible space groups with Bravais lattice *oP* and Laue class *mmm*; Patterson symmetry *Pmmm*

Reflection conditions						Space group	No.	Space group	No.	Space group	No.
0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*						
						***P*222** *P*2*mm*	16 25	*Pmm*2 *Pmmm*	25 47	*Pm*2*m*	25
					l	***P*222$_1$**	17				
				k		***P*22$_1$2**	17				
				k	*l*	***P*22$_1$2$_1$**	18				
			h			***P*2$_1$22**	17				
			h		*l*	***P*2$_1$22$_1$**	18				
			h	*k*		***P*2$_1$2$_1$2**	18				
			h	*k*	*l*	***P*2$_1$2$_1$2$_1$**	19				
		h	*h*			*P*2$_1$*ma*	26	*Pm*2*a*	28	*Pmma*	51
		k		*k*		*Pm*2$_1$*b*	26	*P*2*mb*	28	*Pmmb*	51
		h + *k*	*h*	*k*		*Pm*2$_1$*n*	31	*P*2$_1$*mn*	31	*Pmmn*	59
	h		*h*			*P*2$_1$*am*	26	*Pma*2	28	*Pmam*	51
	h	*h*	*h*			*P*2*aa*	27	*Pmaa*	49		
	h	*k*	*h*	*k*		*P*2$_1$*ab*	29	*Pmab*	57		
	h	*h* + *k*	*h*	*k*		*P*2*an*	30	*Pman*	53		
	l				*l*	*Pmc*2$_1$	26	*P*2*cm*	28	*Pmcm*	51
	l	*h*	*h*		*l*	*P*2$_1$*ca*	29	*Pmca*	57		
	l	*k*		*k*	*l*	*P*2*cb*	32	*Pmcb*	55		
	l	*h* + *k*	*h*	*k*	*l*	*P*2$_1$*cn*	33	*Pmcn*	62		
	h + *l*		*h*		*l*	*Pmn*2$_1$	31	*P*2$_1$*nm*	31	*Pmnm*	59
	h + *l*	*h*	*h*		*l*	*P*2*na*	30	*Pmna*	53		
	h + *l*	*k*	*h*	*k*	*l*	*P*2$_1$*nb*	33	*Pmnb*	62		
	h + *l*	*h* + *k*	*h*	*k*	*l*	*P*2*nn*	34	*Pmnn*	58		
k				*k*		*Pb*2$_1$*m*	26	*Pbm*2	28	*Pbmm*	51
k		*h*	*h*	*k*		*Pb*2$_1$*a*	29	*Pbma*	57		
k		*k*		*k*		*Pb*2*b*	27	*Pbmb*	49		
k		*h* + *k*	*h*	*k*		*Pb*2*n*	30	*Pbmn*	53		
k	*h*		*h*	*k*		*Pba*2	32	*Pbam*	55		
k	*h*	*h*	*h*	*k*		*Pbaa*	54				
k	*h*	*k*	*h*	*k*		*Pbab*	54				
k	*h*	*h* + *k*	*h*	*k*		*Pban*	50				
k	*l*			*k*	*l*	*Pbc*2$_1$	29	*Pbcm*	57		
k	*l*	*h*	*h*	*k*	*l*	*Pbca*	61				
k	*l*	*k*		*k*	*l*	*Pbcb*	54				
k	*l*	*h* + *k*	*h*	*k*	*l*	*Pbcn*	60				

Table 1.6.4.7 (continued)

Reflection conditions						Space group	No.	Space group	No.	Space group	No.
0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*						
k	*h* + *l*		*h*	*k*	*l*	*Pbn*2_1	33	*Pbnm*	62		
k	*h* + *l*	*h*	*h*	*k*	*l*	*Pbna*	60				
k	*h* + *l*	*k*	*h*	*k*	*l*	*Pbnb*	56				
k	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*Pbnn*	52				
l					*l*	*Pcm*2_1	26	*Pc*2*m*	28	*Pcmm*	51
l		*h*	*h*		*l*	*Pc*2*a*	32	*Pcma*	55		
l		*k*		*k*	*l*	*Pc*2_1*b*	29	*Pcmb*	57		
l		*h* + *k*	*h*	*k*	*l*	*Pc*2_1*n*	33	*Pcmn*	62		
l	*h*		*h*		*l*	*Pca*2_1	29	*Pcam*	57		
l	*h*	*h*	*h*		*l*	*Pcaa*	54				
l	*h*	*k*	*h*	*k*	*l*	*Pcab*	61				
l	*h*	*h* + *k*	*h*	*k*	*l*	*Pcan*	60				
l	*l*				*l*	*Pcc*2	27	*Pccm*	49		
l	*l*	*h*	*h*		*l*	*Pcca*	54				
l	*l*	*k*		*k*	*l*	*Pccb*	54				
l	*l*	*h* + *k*	*h*	*k*	*l*	*Pccn*	56				
l	*h* + *l*		*h*		*l*	*Pcn*2	30	*Pcnm*	53		
l	*h* + *l*	*h*	*h*		*l*	*Pcna*	50				
l	*h* + *l*	*k*	*h*	*k*	*l*	*Pcnb*	60				
l	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*Pcnn*	52				
k + *l*				*k*	*l*	*Pnm*2_1	31	*Pn*2_1*m*	31	*Pnmm*	59
k + *l*		*h*	*h*	*k*	*l*	*Pn*2_1*a*	33	*Pnma*	62		
k + *l*		*k*		*k*	*l*	*Pn*2*b*	30	*Pnmb*	53		
k + *l*		*h* + *k*	*h*	*k*	*l*	*Pn*2*n*	34	*Pnmn*	58		
k + *l*	*h*		*h*	*k*	*l*	*Pna*2_1	33	*Pnam*	62		
k + *l*	*h*	*h*	*h*	*k*	*l*	*Pnaa*	56				
k + *l*	*h*	*k*	*h*	*k*	*l*	*Pnab*	60				
k + *l*	*h*	*h* + *k*	*h*	*k*	*l*	*Pnan*	52				
k + *l*	*l*			*k*	*l*	*Pnc*2	30	*Pncm*	53		
k + *l*	*l*	*h*	*h*	*k*	*l*	*Pnca*	60				
k + *l*	*l*	*k*		*k*	*l*	*Pncb*	50				
k + *l*	*l*	*h* + *k*	*h*	*k*	*l*	*Pncn*	52				
k + *l*	*h* + *l*		*h*	*k*	*l*	*Pnn*2	34	*Pnnm*	58		
k + *l*	*h* + *l*	*h*	*h*	*k*	*l*	*Pnna*	52				
k + *l*	*h* + *l*	*k*	*h*	*k*	*l*	*Pnnb*	52				
k + *l*	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*Pnnn*	48				

Table 1.6.4.8
Reflection conditions and possible space groups with Bravais lattice *oS* (*oC* setting) and Laue class *mmm*; Patterson symmetry *Cmmm*

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*						
$h + k$	k	h	$h + k$	h	k		***C*222** *C*2*mm*	21 38	*Cmm*2 *Cmmm*	35 65	*Cm*2*m*	38
$h + k$	k	h	$h + k$	h	k	l	***C*222$_1$**	20				
$h + k$	k	h	h, k	h	k		*Cm*2*e*	39	*C*2*me*	39	*Cme*	67
$h + k$	k	h, l	$h + k$	h	k	l	*Cmc*2$_1$	36	*C*2*cm*	40	*Cmcm*	63
$h + k$	k	h, l	h, k	h	k	l	*C*2*ce*	41	*Cmce*	64		
$h + k$	k, l	h	$h + k$	h	k	l	*Ccm*2$_1$	36	*Cc*2*m*	40	*Ccmm*	63
$h + k$	k, l	h	h, k	h	k	l	*Cc*2*e*	41	*Ccme*	64		
$h + k$	k, l	h, l	$h + k$	h	k	l	*Ccc*2	37	*Cccm*	66		
$h + k$	k, l	h, l	h, k	h	k	l	*Ccce*	68				

Table 1.6.4.9
Reflection conditions and possible space groups with Bravais lattice *oS* (*oB* setting) and Laue class *mmm*; Patterson symmetry *Bmmm*

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*						
$h + l$	l	$h + l$	h	h		l	***B*222** *B*2*mm*	21 38	*Bm*2*m* *Bmmm*	35 65	*Bmm*2	38
$h + l$	l	$h + l$	h	h	k	l	***B*22$_1$2**	20				
$h + l$	l	$h + l$	h, k	h	k	l	*Bm*2$_1$*b*	36	*B*2*mb*	40	*Bmmb*	63
$h + l$	l	h, l	h	h		l	*Bme*2	39	*B*2*em*	39	*Bmem*	67
$h + l$	l	h, l	h, k	h	k	l	*B*2*eb*	41	*Bmeb*	64		
$h + l$	k, l	$h + l$	h	h	k	l	*Bb*2$_1$*m*	36	*Bbm*2	40	*Bbmm*	63
$h + l$	k, l	$h + l$	h, k	h	k	l	*Bb*2*b*	37	*Bbmb*	66		
$h + l$	k, l	h, l	h	h	k	l	*Bbe*2	41	*Bbem*	64		
$h + l$	k, l	h, l	h, k	h	k	l	*Bbeb*	68				

Table 1.6.4.10
Reflection conditions and possible space groups with Bravais lattice *oS* (*oA* setting) and Laue class *mmm*; Patterson symmetry *Ammm*

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*						
$k + l$	$k + l$	l	k		k	l	***A*222** *Amm*2	21 38	*A*2*mm* *Ammm*	35 65	*Am*2*m*	38
$k + l$	$k + l$	l	k	h	k	l	***A*2$_1$22**	20				
$k + l$	$k + l$	l	h, k	h	k	l	*A*2$_1$*ma*	36	*Am*2*a*	40	*Amma*	63
$k + l$	$k + l$	h, l	k	h	k	l	*A*2$_1$*am*	36	*Ama*2	40	*Amam*	63
$k + l$	$k + l$	h, l	h, k	h	k	l	*A*2*aa*	37	*Amaa*	66		
$k + l$	k, l	l	k		k	l	*Aem*2	39	*Ae*2*m*	39	*Aemm*	67
$k + l$	k, l	l	h, k	h	k	l	*Ae*2*a*	41	*Aema*	64		
$k + l$	k, l	h, l	k	h	k	l	*Aea*2	41	*Aeam*	64		
$k + l$	k, l	h, l	h, k	h	k	l	*Aeaa*	68				

Table 1.6.4.11
Reflection conditions and possible space groups with Bravais lattice *oI* and Laue class *mmm*; Patterson symmetry *Immm*

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*						
$h+k+l$	$k+l$	$h+l$	$h+k$	h	k	l	***I*222** *Im*2*m*	23 44	$\boldsymbol{I2_12_12_1}$ *I*2*mm*	24 44	*Imm*2 *Immm*	44 71
$h+k+l$	$k+l$	$h+l$	h, k	h	k	l	*Im*2*a* *Immb*	46 74	*I*2*mb*	46	*Imma*	74
$h+k+l$	$k+l$	h, l	$h+k$	h	k	l	*Ima*2 *Imcm*	46 74	*I*2*cm*	46	*Imam*	74
$h+k+l$	$k+l$	h, l	h, k	h	k	l	*I*2*cb*	45	*Imcb*	72		
$h+k+l$	k, l	$h+l$	$h+k$	h	k	l	*Ibm*2 *Icmm*	46 74	*Ic*2*m*	46	*Ibmm*	74
$h+k+l$	k, l	$h+l$	h, k	h	k	l	*Ic*2*a*	45	*Icma*	72		
$h+k+l$	k, l	h, l	$h+k$	h	k	l	*Iba*2	45	*Ibam*	72		
$h+k+l$	k, l	h, l	h, k	h	k	l	*Ibca*	73	*Icab*	73		

Table 1.6.4.12
Reflection conditions and possible space groups with Bravais lattice *oF* and Laue class *mmm*; Patterson symmetry *Fmmm*

Reflection conditions							Space group	No.
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*		
$h+k, h+l, k+l$	k, l	h, l	h, k	h	k	l	***F*222** *Fmm*2 *Fm*2*m* *F*2*mm* *Fmmm*	22 42 42 42 69
$h+k, h+l, k+l$	k, l	$h+l=4n; h, l$	$h+k=4n; h, k$	$h=4n$	$k=4n$	$l=4n$	*F*2*dd*	43
$h+k, h+l, k+l$	$k+l=4n; k, l$	h, l	$h+k=4n; h, k$	$h=4n$	$k=4n$	$l=4n$	*Fd*2*d*	43
$h+k, h+l, k+l$	$k+l=4n; k, l$	$h+l=4n; h, l$	h, k	$h=4n$	$k=4n$	$l=4n$	*Fdd*2	43
$h+k, h+l, k+l$	$k+l=4n; k, l$	$h+l=4n; h, l$	$h+k=4n; h, k$	$h=4n$	$k=4n$	$l=4n$	*Fddd*	70

Table 1.6.4.13
Reflection conditions and possible space groups with Bravais lattice *tP* and Laue class 4/*m*; *hk* are permutable; Patterson symmetry *P*4/*m*

Reflection conditions					Space group	No.	Space group	No.	Space group	No.
*hk*0	0*kl*	$h \pm h\, l$	00*l*	*h*00						
					***P*4**	75	$P\bar{4}$	81	$P4/m$	83
			l		$\boldsymbol{P4_2}$	77	$P4_2/m$	84		
			$l=4n$		$\boldsymbol{P4_1}$	76	$\boldsymbol{P4_3}$	78		
$h+k$				h	$P4/n$	85				
$h+k$			l	h	$P4_2/n$	86				

Table 1.6.4.14
Reflection conditions and possible space groups with Bravais lattice *tP* and Laue class 4/*mmm*; *hk* are permutable; Patterson symmetry *P*4/*mmm*

Reflection conditions					Space group	No.	Space group	No.	Space group	No.
*hk*0	0*kl*	*h* ± *h l*	00*l*	*h*00						
					***P*422**	89	*P*4*mm*	99	$P\bar{4}2m$	111
					$P\bar{4}m2$	115	*P*4/*mmm*	123		
				h	***P*42$_1$2**	90	$P\bar{4}2_1m$	113		
			l		***P*4$_2$22**	93				
			l	*h*	***P*4$_2$2$_1$2**	94				
			l = 4*n*		***P*4$_1$22**	91	***P*4$_3$22**	95		
			l = 4*n*	*h*	***P*4$_1$2$_1$2**	92	***P*4$_3$2$_1$2**	96		
		l	*l*		*P*4$_2$*mc*	105	$P\bar{4}2c$	112	*P*4$_2$/*mmc*	131
		l	*l*	*h*	$P\bar{4}2_1c$	114				
	k			*h*	*P*4*bm*	100	$P\bar{4}b2$	117	*P*4/*mbm*	127
	k	*l*	*l*	*h*	*P*4$_2$*bc*	106	*P*4$_2$/*mbc*	135		
	l		*l*		*P*4$_2$*cm*	101	$P\bar{4}c2$	116	*P*4$_2$/*mcm*	132
	l	*l*	*l*		*P*4*cc*	103	*P*4/*mcc*	124		
	k + *l*		*l*	*h*	*P*4$_2$*nm*	102	$P\bar{4}n2$	118	*P*4$_2$/*mnm*	136
	k + *l*	*l*	*l*	*h*	*P*4*nc*	104	*P*4/*mnc*	128		
h + *k*				*h*	*P*4/*nmm*	129				
h + *k*		*l*	*l*	*h*	*P*4$_2$/*nmc*	137				
h + *k*	*k*			*h*	*P*4/*nbm*	125				
h + *k*	*k*	*l*	*l*	*h*	*P*4$_2$/*nbc*	133				
h + *k*	*l*		*l*	*h*	*P*4$_2$/*ncm*	138				
h + *k*	*l*	*l*	*l*	*h*	*P*4/*ncc*	130				
h + *k*	*k* + *l*		*l*	*h*	*P*4$_2$/*nnm*	134				
h + *k*	*k* + *l*	*l*	*l*	*h*	*P*4/*nnc*	126				

Table 1.6.4.15
Reflection conditions and possible space groups with Bravais lattice *tI* and Laue class 4/*m*; *hk* are permutable; Patterson symmetry *I*4/*m*

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	*hk*0	0*kl*	*h* ± *h l*	00*l*	*h*00	*h* ± *h* 0						
h + *k* + *l*	*h* + *k*	*k* + *l*	*l*	*l*	*h*		***I*4**	79	$I\bar{4}$	82	*I*4/*m*	87
h + *k* + *l*	*h* + *k*	*k* + *l*	*l*	*l* = 4*n*	*h*		***I*4$_1$**	80				
h + *k* + *l*	*h*, *k*	*k* + *l*	*l*	*l* = 4*n*	*h*	*h*	*I*4$_1$/*a*	88				

Table 1.6.4.16
Reflection conditions and possible space groups with Bravais lattice *tI* and Laue class 4/*mmm*; *hk* are permutable; Patterson symmetry *I*4/*mmm*

Reflection conditions							Space group	No.	Space group	No.	Space group	No.
hkl	*hk*0	0*kl*	$h \pm h\, l$	00*l*	*h*00	$h \pm h\, 0$						
$h+k+l$	$h+k$	$k+l$	l	l	h		**I422** $I\bar{4}2m$	97 121	$I4mm$ $I4/mmm$	107 139	$I\bar{4}m2$	119
$h+k+l$	$h+k$	$k+l$	l	$l=4n$	h		$\mathbf{I4_122}$	98				
$h+k+l$	$h+k$	$k+l$	$2h+l=4n$	$l=4n$	h	h	$I4_1md$	109	$I\bar{4}2d$	122		
$h+k+l$	$h+k$	k, l	l	l	h		$I4cm$	108	$I\bar{4}c2$	120	$I4/mcm$	140
$h+k+l$	$h+k$	k, l	$2h+l=4n$	$l=4n$	h	h	$I4_1cd$	110				
$h+k+l$	h, k	$k+l$	$2h+l=4n$	$l=4n$	h	h	$I4_1/amd$	141				
$h+k+l$	h, k	k, l	$2h+l=4n$	$l=4n$	h	h	$I4_1/acd$	142				

Table 1.6.4.17
Reflection conditions and possible space groups with Bravais lattice *hP* and Laue class $\bar{3}$; *hki* are permutable; Patterson symmetry $P\bar{3}$

Reflection conditions			Space group	No.	Space group	No.
$hh\bar{2}hl$	$h\bar{h}0l$	000*l*				
			P3	143	$P\bar{3}$	147
		$l=3n$	$\mathbf{P3_1}$	144	$\mathbf{P3_2}$	145

Table 1.6.4.18
Reflection conditions and possible space groups with Bravais lattice *hP* and Laue classes $\bar{3}1m$ and $\bar{3}m1$; *hki* are permutable; Patterson symmetry $P\bar{3}1m$ and $P\bar{3}m1$

Reflection conditions			Class $\bar{3}1m$		Class $\bar{3}m1$	
$hh\bar{2}hl$	$h\bar{h}0l$	000*l*	Space group	No.	Space group	No.
			P312	149	**P321**	150
			$P31m$	157	$P3m1$	156
			$P\bar{3}1m$	162	$P\bar{3}m1$	164
		$l=3n$	$\mathbf{P3_112}$	151	$\mathbf{P3_121}$	152
			$\mathbf{P3_212}$	153	$\mathbf{P3_221}$	154
l		l	$P31c$	159		
			$P\bar{3}1c$	163		
	l	l			$P3c1$	158
					$P\bar{3}c1$	165

Table 1.6.4.19
Reflection conditions and possible space groups with Bravais lattice *hP* and Laue class 6/*m*; *hki* are permutable; Patterson symmetry *P*6/*m*

Reflection conditions			Space group	No.	Space group	No.	Space group	No.
$hh\bar{2}hl$	$h\bar{h}0l$	000*l*						
			P6	168	$P\bar{6}$	174	$P6/m$	175
		l	$\mathbf{P6_3}$	173	$P6_3/m$	176		
		$l=3n$	$\mathbf{P6_2}$	171	$\mathbf{P6_4}$	172		
		$l=6n$	$\mathbf{P6_1}$	169	$\mathbf{P6_5}$	170		

Table 1.6.4.20
Reflection conditions and possible space groups with Bravais lattice *hP* and Laue class 6/*mmm*; *hki* are permutable; Patterson symmetry *P*6/*mmm*

Reflection conditions			Space group	No.	Space group	No.	Space group	No.
$hh\bar{2}\bar{h}l$	$h\bar{h}0l$	$000l$						
			***P*622**	177	*P*6*mm*	183	$P\bar{6}m2$	187
			$P\bar{6}2m$	189	*P*6/*mmm*	191		
		l	$\boldsymbol{P6_322}$	182				
		$l = 3n$	$\boldsymbol{P6_222}$	180	$\boldsymbol{P6_422}$	181		
		$l = 6n$	$\boldsymbol{P6_122}$	178	$\boldsymbol{P6_522}$	179		
l		l	$P6_3mc$	186	$P\bar{6}2c$	190	$P6_3/mmc$	194
	l	l	$P6_3cm$	185	$P\bar{6}c2$	188	$P6_3/mcm$	193
l	l	l	*P*6*cc*	184	*P*6/*mcc*	192		

Table 1.6.4.21
Reflection conditions and possible space groups with Bravais lattice *hR* and Laue class $\bar{3}$ (hexagonal axes); *hki* are permutable; Patterson symmetry $R\bar{3}$; Ov = obverse setting; Rv = reverse setting

Reflection conditions						Space group	No.	Space group	No.	
hkil	*hki*0	$hh\bar{2}\bar{h}l$	$h\bar{h}0l$	$000l$	$h\bar{h}00$					
$-h+k+l=3n$	$-h+k=3n$	$l=3n$	$h+l=3n$	$l=3n$	$h=3n$	***R*3**	146	$R\bar{3}$	148	Ov
$h-k+l=3n$	$h-k=3n$	$l=3n$	$-h+l=3n$	$l=3n$	$h=3n$	***R*3**	146	$R\bar{3}$	148	Rv

Table 1.6.4.22
Reflection conditions and possible space groups with Bravais lattice *hR* and Laue class $\bar{3}m$ (hexagonal axes); *hki* are permutable; Patterson symmetry $R\bar{3}m$; Ov = obverse setting; Rv = reverse setting

Reflection conditions						Space group	No.	Space group	No.	Space group	No.	
hkil	*hki*0	$hh\bar{2}\bar{h}l$	$h\bar{h}0l$	$000l$	$h\bar{h}00$							
$-h+k+l=3n$	$-h+k=3n$	$l=3n$	$h+l=3n$	$l=3n$	$h=3n$	***R*32**	155	*R*3*m*	160	$R\bar{3}m$	166	Ov
$-h+k+l=3n$	$-h+k=3n$	$l=3n$	$h+l=3n, l=2m$	$l=6n$	$h=3n$	*R*3*c*	161	$R\bar{3}c$	167			Ov
$h-k+l=3n$	$h-k=3n$	$l=3n$	$-h+l=3n$	$l=3n$	$h=3n$	***R*32**	155	*R*3*m*	160	$R\bar{3}m$	166	Rv
$h-k+l=3n$	$h-k=3n$	$l=3n$	$-h+l=3n, l=2m$	$l=6n$	$h=3n$	*R*3*c*	161	$R\bar{3}c$	167			Rv

Table 1.6.4.23
Reflection conditions and possible space groups with Bravais lattice *hR* and Laue class $\bar{3}$ (rhombohedral axes); *hkl* are permutable; Patterson symmetry $R\bar{3}$

Reflection conditions		Space group	No.	Space group	No.
hhl	*hhh*				
		***R*3**	146	$R\bar{3}$	148

Table 1.6.4.24
Reflection conditions and possible space groups with Bravais lattice *hR* and Laue class $\bar{3}m$ (rhombohedral axes); *hkl* are permutable; Patterson symmetry $R\bar{3}m$

Reflection conditions		Space group	No.	Space group	No.	Space group	No.
hhl	*hhh*						
		***R*32**	155	*R*3*m*	160	$R\bar{3}m$	166
l	h	*R*3*c*	161	$R\bar{3}c$	167		

Table 1.6.4.25
Reflection conditions and possible space groups with Bravais lattice *cP* and Laue class $m\bar{3}$; *hkl* are cyclically permutable; Patterson symmetry $Pm\bar{3}$

Reflection conditions			Space group	No.	Space group	No.
$0kl$	$h \pm h\,l$	$h00$				
			***P*23**	195	$Pm\bar{3}$	200
		h	***P*2$_1$3**	198		
k		h	$Pa\bar{3}$	205		
l		h	$Pb\bar{3}$	205		
$k + l$		h	$Pn\bar{3}$	201		

Table 1.6.4.26
Reflection conditions and possible space groups with Bravais lattice *cP* and Laue class $m\bar{3}m$; *hkl* are permutable; Patterson symmetry $Pm\bar{3}m$

Reflection conditions			Space group	No.	Space group	No.	Space group	No.
$0kl$	$h \pm h\,l$	$h00$						
			***P*432**	207	$P\bar{4}3m$	215	$Pm\bar{3}m$	221
		h	***P*4$_2$32**	208				
		$h = 4n$	***P*4$_3$32**	212	***P*4$_1$32**	213		
	l	h	$P\bar{4}3n$	218	$Pm\bar{3}n$	223		
$k + l$		h	$Pn\bar{3}m$	224				
$k + l$	l	h	$Pn\bar{3}n$	222				

Table 1.6.4.27
Reflection conditions and possible space groups with Bravais lattice *cI* and Laue class $m\bar{3}$; *hkl* are cyclically permutable; Patterson symmetry $Im\bar{3}$

Reflection conditions				Space group	No.	Space group	No.	Space group	No.
hkl	$0kl$	$h \pm h\,l$	$h00$						
$h + k + l$	$k + l$	l	h	***I*23**	197	***I*2$_1$3**	199	$Im\bar{3}$	204
$h + k + l$	k, l	l	h	$Ia\bar{3}$	206				

Table 1.6.4.28
Reflection conditions and possible space groups with Bravais lattice *cI* and Laue class $m\bar{3}m$; *hkl* are permutable; Patterson symmetry $Im\bar{3}m$

Reflection conditions				Space group	No.	Space group	No.	Space group	No.
hkl	$0kl$	$h \pm h\,l$	$h00$						
$h + k + l$	$k + l$	l	h	***I*432**	211	$I\bar{4}3m$	217	$Im\bar{3}m$	229
$h + k + l$	$k + l$	l	$h = 4n$	***I*4$_1$32**	214				
$h + k + l$	$k + l$	$2h + l = 4n$	$h = 4n$	$I\bar{4}3d$	220				
$h + k + l$	k, l	$2h + l = 4n$	$h = 4n$	$Ia\bar{3}d$	230				

Table 1.6.4.29
Reflection conditions and possible space groups with Bravais lattice *cF* and Laue class $m\bar{3}$; *hkl* are cyclically permutable; Patterson symmetry $Fm\bar{3}$

Reflection conditions				Space group	No.	Space group	No.
hkl	$0kl$	$h \pm h\,l$	$h00$				
$h + k, h + l, k + l$	k, l	$h + l$	h	***F*23**	196	$Fm\bar{3}$	202
$h + k, h + l, k + l$	$k + l = 4n; k, l$	$h + l$	$h = 4n$	$Fd\bar{3}$	203		

Table 1.6.4.30
Reflection conditions and possible space groups with Bravais lattice *cF* and Laue class $m\bar{3}m$; *hkl* are permutable; Patterson symmetry $Fm\bar{3}m$

Reflection conditions				Space group	No.	Space group	No.	Space group	No.
hkl	0*kl*	$h \pm hl$	*h*00						
$h+k, h+l, k+l$	k, l	$h+l$	h	***F*432**	209	$F\bar{4}3m$	216	$Fm\bar{3}m$	225
$h+k, h+l, k+l$	k, l	$h+l$	$h=4n$	***F*4$_1$32**	210				
$h+k, h+l, k+l$	k, l	h, l	h	$F\bar{4}3c$	219	$Fm\bar{3}c$	226		
$h+k, h+l, k+l$	$k+l=4n; k, l$	$h+l$	$h=4n$	$Fd\bar{3}m$	227				
$h+k, h+l, k+l$	$k+l=4n; k, l$	h, l	$h=4n$	$Fd\bar{3}c$	228				

and have not yet enjoyed widespread distribution, use and acceptance by the community. Flack *et al.* (2011) and Parsons *et al.* (2012) give detailed information on these calculations.

1.6.5.1.2. Status of centrosymmetry and resonant scattering

The basic starting point in this analysis is the following linear transformation of $|F(hkl)|^2$ and $|F(\overline{hkl})|^2$, applicable to both observed and model values, to give the average (A) and difference (D) intensities:

$$A(hkl) = \tfrac{1}{2}[|F(hkl)|^2 + |F(\overline{hkl})|^2],$$
$$D(hkl) = |F(hkl)|^2 - |F(\overline{hkl})|^2.$$

In equation (1.6.2.1), $A(hkl)$ was denoted by $|F_{\rm av}(hkl)|^2$. The expression for $D(hkl)$ corresponding to that for $A(hkl)$ given in equation (1.6.2.1) and using the same nomenclature is

$$D(\mathbf{h}) = \sum_{i,j}[(f_i + f_i')f_j'' - (f_j + f_j')f_i'']\sin[2\pi\mathbf{h}(\boldsymbol{r}_i - \boldsymbol{r}_j)].$$

In general $|D(hkl)|$ is small compared to $A(hkl)$. A compound with an appreciable resonant-scattering contribution has $|D(hkl)| \approx 0.01A(hkl)$, whereas a compound with a small resonant-scattering contribution has $|D(hkl)| \approx 0.0001A(hkl)$. For centric reflections, $D_{\rm model} = 0$, and so the values of $D_{\rm obs}(hkl)$ of these are entirely due to random uncertainties and systematic errors in the intensity measurements. $D_{\rm obs}(hkl)$ of acentric reflections contains contributions both from the random uncertainties and the systematic errors of the data measurements, and from the differences between $|F(hkl)|^2$ and $|F(\overline{hkl})|^2$ which arise through the effect of resonant scattering. A slight experimental limitation is that a data set of intensities needs to contain both reflections *hkl* and $\overline{hkl}$ in order to obtain $A_{\rm obs}(hkl)$ and $D_{\rm obs}(hkl)$.

The Bijvoet ratio, defined by

$$\chi = \frac{\langle D^2\rangle^{1/2}}{\langle A\rangle},$$

is the ratio of the root-mean-square value of D to the mean value of A. In a structure analysis, two independent estimates of the Bijvoet ratio are available and their comparison leads to useful information as to whether the crystal structure is centrosymmetric or not.

The first estimate arises from considerations of intensity statistics leading to the definition of the Bijvoet ratio as a value called Friedif$_{\rm stat}$, whose functional form was derived by Flack & Shmueli (2007) and Shmueli & Flack (2009). One needs only to know the chemical composition of the compound and the wavelength of the X-radiation to calculate Friedif$_{\rm stat}$ using various available software.

The second estimate of the Bijvoet ratio, Friedif$_{\rm obs}$, is obtained from the observed diffraction intensities. One problematic point in the evaluation of Friedif$_{\rm obs}$ arises because A and D do not have the same dependence on $\sin\theta/\lambda$ and it is necessary to eliminate this difference as far as possible. A second problematic point in the calculation is to make sure that only acentric reflections of any of the noncentrosymmetric point groups in the chosen Laue class are selected for the calculation of Friedif$_{\rm obs}$. In this way one is sure that if the point group of the crystal is centrosymmetric, all of the chosen reflections are centric, and if the point group of the crystal is noncentrosymmetric, all of the chosen reflections are acentric. The necessary selection is achieved by taking only those reflections that are general in the Laue group. To date (2015), the calculation of Friedif$_{\rm obs}$ is not available in distributed software. On comparison of Friedif$_{\rm stat}$ with Friedif$_{\rm obs}$, one is able to state with some confidence that:

(1) if Friedif$_{\rm obs}$ is much lower than Friedif$_{\rm stat}$, then the crystal structure is either centrosymmetric, and random uncertainties and systematic errors in the data set are minor, or noncentrosymmetric with the crystal twinned by inversion in a proportion close to 50:50;
(2) if Friedif$_{\rm obs}$ is close in value to Friedif$_{\rm stat}$, then the crystal is probably noncentrosymmetric and random uncertainties and systematic errors in the data set are minor. However, data from a centrosymmetric crystal with large random uncertainties and systematic errors may also produce this result; and
(3) if Friedif$_{\rm obs}$ is much larger than Friedif$_{\rm stat}$ then either the data set is dominated by random uncertainties and systematic errors or the chemical formula is erroneous.

Example 1

The crystal of compound Ex1 (Udupa & Krebs, 1979) is known to be centrosymmetric (space group $P2_1/c$) and has a significant resonant-scattering contribution, Friedif$_{\rm stat}$ = 498 and Friedif$_{\rm obs}$ = 164. The comparison of Friedif$_{\rm stat}$ and Friedif$_{\rm obs}$ indicates that the crystal structure is centrosymmetric.

Example 2

The crystal of compound Ex2, potassium hydrogen (2*R*,3*R*) tartrate, is known to be enantiomerically pure and appears in space group $P2_12_12_1$. The value of Friedif$_{\rm obs}$ is 217 compared to a Friedif$_{\rm stat}$ value of 174. The agreement is good and allows the deduction that the crystal is neither centrosymmetric, nor twinned by inversion in a proportion near to 50:50, nor that the

Table 1.6.5.1
R_{merge} values for Ex2 for the 589 sets of general reflections of *mmm* which have all eight measurements in the set

R_{merge} (%)	*mmm*	2*mm*	*m*2*m*	*mm*2	222
R_A	1.30	1.30	1.30	1.30	1.30
R_D	100.0	254.4	235.7	258.1	82.9

Table 1.6.5.2
R_{merge} values for Ex1 for the 724 sets of general reflections of 2/*m* which have all four measurements in the set

R_{merge} (%)	2/*m*	*m*	2
R_A	1.29	1.29	1.29
R_D	100.0	98.3	101.7

data set is unsatisfactorily dominated by random uncertainty and systematic error.

Example 3

The crystals of compound Ex3 (Zhu & Jiang, 2007) occur in Laue group $\overline{1}$. One finds Friedif_{stat} = 70 and Friedif_{obs} = 499. The huge discrepency between the two shows that the observed values of D are dominated by random uncertainty and systematic error.

1.6.5.1.3. Resolution of noncentrosymmetric ambiguities

It was shown in Section 1.6.5.1.2 that under certain circumstances it is possible to determine whether or not the space group of the crystal investigated is centrosymmetric. Suppose that the space group was found to be noncentrosymmetric. In each Laue class, there is one centrosymmetric point group and one or more noncentrosymmetric point groups. For example, in the Laue class *mmm* we need to distinguish between the point groups 222, 2*mm*, *m*2*m* and *mm*2, and of course between the space groups based on them. We shall show that it is possible in practice to distinguish between these noncentrosymmetric point groups using intensity differences between Friedel opposites caused by resonant scattering.

An excellent intensity data set from a crystal (Ex2 above) of potassium hydrogen (2*R*, 3*R*) tartrate, measured with a wavelength of 0.7469 Å at 100 K, was used. The Laue group was assumed to be *mmm*. The raw data set was initially merged and averaged in point group 1 and all special reflections of the Laue group *mmm* (*i.e.* 0*kl*, *h*0*l*, *hk*0, *h*00, 0*k*0, 00*l*) were set aside. The remaining data were organized into sets of reflections symmetry-equivalent under the Laue group *mmm*, and only those sets (589 in all) containing all 8 of the *mmm*-symmetry-equivalent reflections were retained. Each of these sets provides 4 A_{obs} and 4 D_{obs} values which can be used to calculate R_{merge} values appropriate to the five point groups in the Laue class *mmm*. The results are given in Table 1.6.5.1. The value of 100% for R_{merge} in a centrosymmetric point group, such as *mmm* or 2/*m*, arises by definition and not by coincidence. The R_D of the true point group has the lowest value, which is noticeably different from the other choices of point group.

The crystal of Ex1 above (space group $P2_1/c$) was treated in a similar manner. Table 1.6.5.2 shows that R_D values display no preference between the three point groups in Laue class 2/*m*.

Intensity measurements comprising a full sphere of reflections are essential to the success of the R_{merge} tests described in this section.

1.6.5.1.4. Data evaluation after structure refinement

There is an excellent way in which to evaluate both data measurement and treatment procedures, and the fit of the model to the data, including the space-group assignment, at the completion of structure refinement. This technique is applicable both to noncentrosymmetric and to centrosymmetric crystals. A scattergram of D_{obs} against D_{model}, and $2A_{obs}$ against $2A_{model}$ pairs are plotted on the same graph. All (D_{obs}, D_{model}) pairs are plotted together with those ($2A_{obs}$, $2A_{model}$) pairs which have $2A_{obs} < |D_{obs}|_{max}$. The range of values on the axes of the model and of the observed values should be identical. For acentric reflections, for both A and D, a good fit of the observed to the model quantities shows itself as a straight line of slope 1 passing through the origin, with some scatter about this ideal straight line. For an individual reflection, 2A and D are, respectively, the sum and the difference of the same quantities and they have identical standard uncertainties. It is thus natural to select 2A and D to plot on the same graph. In practice one sees that the spread of the 2A plot increases with increasing value of 2A. Fig. 1.6.5.1 shows the 2AD plot for Ex2 of Example 2 in Section 1.6.5.1.2, which is most satisfactory and confirms the choice of point group from the use of R_{merge}. The conventional R value for all reflections is 3.1% and for those shown in Fig. 1.6.5.1 it is 10.4%. The R value for all D values is good at 51.1%. Fig. 1.6.5.2 shows the 2AD plot for Ex1 of Example 1 in Section 1.6.5.1.2. The structure model is centrosymmetric so all D_{model} values are zero. The conventional R value on A for all reflections is 4.3% and for those shown in Fig. 1.6.5.2 it is 9.1%. The R value on all the D values is 100%.

1.6.5.2. Space-group determination in macromolecular crystallography

For macromolecular crystallography, succinct descriptions of space-group determination have been given by Kabsch (2010*a*,*b*, 2012) and Evans (2006, 2011). Two characteristics of macromolecular crystals give rise to variations on the small-molecule procedures described above.

The first characteristic is the large size of the unit cell of macromolecular crystals and the variation of the cell dimensions from one crystal to another. This makes the determination of the Bravais lattice by cell reduction problematic, as small changes of cell dimensions give rise to differences in the assignment. Kabsch (2010*a*,*b*, 2012) uses a 'quality index' from each of Niggli's 44 lattice characters to come to a best choice. Grosse-Kunstleve *et al.* (2004) and Sauter *et al.* (2004) have found that some commonly used methods to determine the Bravais lattice are susceptible to numerical instability, making it possible for high-symmetry Bravais lattice types to be improperly identified. Sauter *et al.* (2004, 2006) find from practical experience that a deviation δ as high as 1.4° from perfect alignment of direct and reciprocal lattice rows must be allowed to construct the highest-symmetry Bravais type consistent with the data. Evans (2006) uses a value of 3.0°. The large unit-cell size also gives rise to a large number of reflections in the asymmetric region of reciprocal space, and taken with the tendency of macromolecular crystals to decompose in the X-ray beam, full-sphere data sets are uncommon. This means that confirmation of the Laue class by means of values of R_{int} (R_{merge}) are rarer than with small-molecule crystallography, although Kabsch (2010*b*) does use a 'redundancy-independent R factor'. Evans (2006, 2011) describes methods very similar to those given as the second stage in Section 1.6.2.1. The conclusion of Sauter *et al.* (2006) and Evans (2006) is that R_{int} values as high

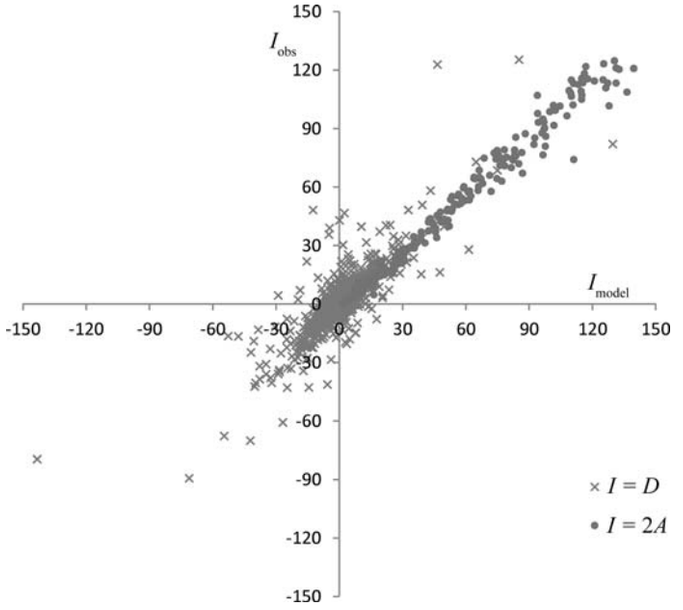

Figure 1.6.5.1
Data-evaluation plot for crystal Ex2. The plot shows a scattergram of all (D_{obs}, D_{model}) pairs and those ($2A_{obs}$, $2A_{model}$) pairs in the same intensity range as the D values.

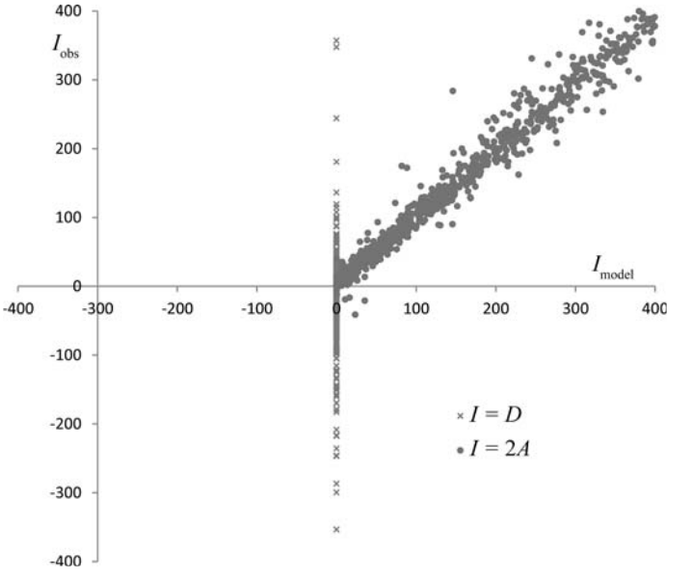

Figure 1.6.5.2
Data-evaluation plot for crystal Ex1. The plot shows a scattergram of all (D_{obs}, D_{model}) and some ($2A_{obs}$, $2A_{model}$) data points.

as 25% must be permitted in order to assemble an optimal set of operations to describe the diffraction symmetry. Another interesting procedure, accompanied by experimental proof, has been devised by Sauter *et al.* (2006). They show that it is clearer to calculate R_{merge} values individually for each potential symmetry operation of a target point group rather than comparing R_{merge} values for target point groups globally. According to Sauter *et al.* (2006) the reason for this improvement lies in the lack of intensity data relating some target symmetry operations.

The second characteristic of macromolecular crystals is that the compound is known, or presumed, to be chiral and enantiomerically pure, so that the crystal structure is chiral. This limits the choice of space group to the 65 Sohncke space groups containing only translations, pure rotations or screw rotations. For ease of use, these have been typeset in bold in Tables 1.6.4.2–1.6.4.30.

For the evaluation of protein structures, Poon *et al.* (2010) apply similar techniques to those described in Section 1.6.2.3. The major tactical objective is to identify pairs of α-helices that have been declared to be symmetry-independent in the structure solution but which may well be related by a rotational symmetry of the crystal structure. Poon *et al.* (2010) have been careful to test their methodology against generated structural data before proceeding to tests on real data. Their results indicate that some 2% of X-ray structures in the Protein Data Bank potentially fit in a higher-symmetry space group. Zwart *et al.* (2008) have studied the problems of under-assigned translational symmetry operations, suspected incorrect symmetry and twinned data with ambiguous space-group choices, and give illustrations of the uses of group–subgroup relations.

1.6.5.3. Space-group determination from powder diffraction

In powder diffraction, the reciprocal lattice is projected onto a single dimension. This projection gives rise to the major difficulty in interpreting powder-diffraction patterns. Reflections overlap each other either exactly, owing to the symmetry of the lattice metric, or approximately. This makes the extraction of the integrated intensities of individual Bragg reflections liable to error. Experimentally, the use of synchrotron radiation with its exceedingly fine and highly monochromatic beam has enabled considerable progress to be made over recent years. Other obstacles to the interpretation of powder-diffraction patterns, which occur at all stages of the analysis, are background interpretation, preferred orientation, pseudo-translational symmetry and impurity phases. These are general powder-diffraction problems and will not be treated at all in the current chapter. The reader should consult David *et al.* (2002) and David & Shankland (2008) or the forthcoming new volume of *International Tables for Crystallography* (Volume H, *Powder Diffraction*) for further information.

It goes without saying that the main use of the powder method is in structural studies of compounds for which single crystals cannot be grown.

Let us start by running through the three stages of extraction of symmetry information from the diffraction pattern described in Section 1.6.2.1 to see how they apply to powder diffraction.

(1) Stage 1 concerns the determination of the Bravais lattice from the experimentally determined cell dimensions. As such, this process is identical to that described in Section 1.6.2.1. The obstacle, arising from peak overlap, is the initial indexing of the powder pattern and the determination of a unit cell, see David *et al.* (2002) and David & Shankland (2008).

(2) Stage 2 concerns the determination of the point-group symmetry of the intensities of the Bragg reflections. As a preparation to stages 2 and 3, the integrated Bragg intensities have to be extracted from the powder-diffraction pattern by one of the commonly used profile analysis techniques [see David *et al.* (2002) and David & Shankland (2008)]. The intensities of severely overlapped reflections are subject to error. Moreover, the exact overlap of reflections owing to the symmetry of the lattice metric makes it impossible to distinguish between high- and low-symmetry Laue groups in the same family *e.g.* between 4/*m* and 4/*mmm* in the tetragonal family and $m\bar{3}$ and $m\bar{3}m$ in the cubic family. Likewise,

differences in intensity between Friedel opposites, *hkl* and $\overline{hkl}$, are hidden in a powder-diffraction pattern and the techniques of Section 1.6.5.1 are inapplicable. It is also known that experimental results on structure-factor statistics described in Section 1.6.2.2 are sensitive to the algorithm used to extract the integrated Bragg intensities from the powder-diffraction pattern. One procedure tends to produce intensity statistics typical of the noncentrosymmetric space group $P1$ and another those of the centrosymmetric space group $P\overline{1}$. In all, nothing much can be learnt from stage 2 for a powder-diffraction pattern. As a consequence, space-group determination from powder diffraction relies entirely on the Bravais lattice derived from the indexing of the diffraction pattern in stage 1 and the detection of systematic absences in stage 3.

(3) Stage 3 concerns the identification of the conditions for possible systematic absences. However, Bragg-peak overlap causes difficulties with determining systematic absences. For powder-diffraction peaks at small values of $\sin\theta/\lambda$, the problem is rarely severe, even for low-resolution laboratory powder-diffraction data. Potentially absent reflections at higher values of $\sin\theta/\lambda$ often overlap with other reflections of observable intensity. Accordingly, conclusions about the presence of space-group symmetry operations are generally drawn on the basis of a very small number of clear intensity observations. Observing lattice-centring absences is usually relatively easy. In the case of molecular organic materials, considerable help in space-group selection comes from the well known frequency distribution of space groups, where some 80% of compounds crystallize in one of the following: $P2_1/c$, $P\overline{1}$, $P2_12_12_1$, $P2_1$ and $C2/c$. Practical methods of proceeding are described by David & Sivia (2002). It should also be pointed out that Table 1.6.4.1 in this chapter may often be found to be helpful. For example, if it is known that the Bravais lattice is of type *cP*, Table 1.6.4.1 tells us that the possible Laue classes are $m\overline{3}$ and $m\overline{3}m$ and the possible space groups can be found in Tables 1.6.4.25 and 1.6.4.26, respectively. The appropriate reflection conditions are of course given in these tables. All relevant tables can thus be located with the aid of Table 1.6.4.1 if the Bravais lattice is known.

There has been considerable progress since 2000 in the automated extraction by software of the set of conditions for reflections from a powder-diffraction pattern for undertaking stage 3 above. Once the conditions have been identified, Tables 1.6.4.2–1.6.4.30 are used to identify the corresponding space groups. The output of such software consists of a ranked list of complete sets of conditions for reflections (*i.e.* the horizontal rows of conditions given in Tables 1.6.4.2–1.6.4.30). Accordingly, the best-ranked set of conditions is at the top of the list followed by others in decreasing order of appropriateness. The list thus is answering the question: Which is the most probable set of reflection conditions for the data to hand? Such software uses integrated intensities of Bragg reflections extracted from the powder pattern and, as mentioned above, the results are sensitive to the particular profile integration procedure used. Moreover, only ideal Wilson (1949) p.d.f.'s for space groups $P1$ and $P\overline{1}$ are implemented. The art of such techniques is to find appropriate criteria such that the most likely set of reflection conditions is clearly discriminated from any others. Altomare *et al.* (Altomare, Caliandro, Camalli, Cuocci, da Silva *et al.*, 2004; Altomare, Caliandro, Camalli, Cuocci, Giacovazzo *et al.*, 2004; Altomare *et al.*, 2005, 2007, 2009) have used a probabilistic approach combining the probabilities of individual symmetry operations of candidate space groups. The approach is pragmatic and has evolved over several versions of the software. Experience has accumulated through use of the procedure and the discrimination of the software has consequently improved. Markvardsen *et al.* (2001, 2012) commence with an in-depth probabilistic analysis using the concepts of Bayesian statistics which was demonstrated on a few test structures. Later, Markvardsen *et al.* (2008) made software generally available for their approach. Vallcorba *et al.* (2012) have also produced software for space-group determination, but give little information on their algorithm.

1.6.6. Space groups for nanocrystals by electron microscopy

By J. C. H. Spence

The determination of crystal space groups may be achieved by the method of convergent-beam electron microdiffraction (CBED) using a modern transmission electron microscope (TEM). A detailed description of the CBED technique is given by Tanaka (2008) in Section 2.5.3 of Volume B; here we give a brief overview of the capabilities of the method for space-group determination, for completeness. A TEM beam focused to nanometre dimensions allows study of nanocrystals, while identification of noncentrosymmetric crystals is straightforward, as a result of the strong multiple scattering normally present in electron diffraction. (Unlike single scattering, this does not impose inversion symmetry on diffraction patterns, but preserves the symmetry of the sample and its boundaries.) CBED patterns also allow direct determination of screw and glide space-group elements, which produce characteristic absences, despite the presence of multiple scattering, in certain orientations. These absences, which remain for all sample thicknesses and beam energies, may be shown to occur as a result of an elegant cancellation theorem along symmetry-related multiple-scattering paths (Gjønnes & Moodie, 1965). Using all of the above information, most of the 230 space groups can be distinguished by CBED. The remaining more difficult cases (such as space groups that differ only in the location of their symmetry elements) are discussed in Spence & Lynch (1982), Eades (1988), and Saitoh *et al.* (2001). Enantiomorphic pairs require detailed atomistic simulations based on a model, as in the case of quartz (Goodman & Secomb, 1977). Multiple scattering renders Bragg intensities sensitive to structure-factor phases in noncentrosymmetric structures, allowing these to be measured with a tenth of a degree accuracy (Zuo *et al.*, 1993). Unlike X-ray diffraction, electron diffraction is very sensitive to ionicity and bonding effects, especially at low angles, allowing extinction-free charge-density mapping with high accuracy (Zuo, 2004; Zuo *et al.*, 1999). Because of its sensitivity to strain, CBED may also be used to map out local phase transformations which cause space-group changes on the nanoscale (Zuo, 1993; Zhang *et al.*, 2006).

In simplest terms, a CBED pattern is formed by enlarging the incident beam divergence in the transmission diffraction geometry, as first demonstrated G. Mollenstedt in 1937 (Kossel & Mollenstedt, 1942). Bragg spots are then enlarged into discs, and the intensity variation within these discs is studied, in addition to that of the entire pattern, in the CBED method. The intensity variation within a disc displays a complete rocking curve in each of the many diffracted orders, which are simultaneously excited

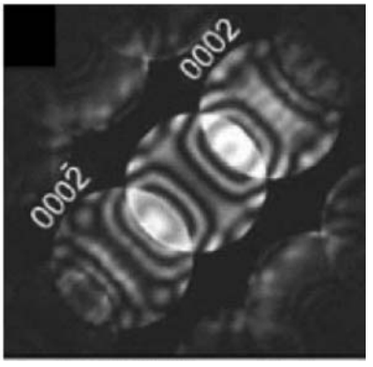

Figure 1.6.6.1
Polarity determination by convergent-beam electron diffraction. A CBED pattern from ZnO with the beam normal to the *c* axis is shown. The intensity distribution along **c** does not have inversion symmetry, reflecting the noncentrocentrosymmetric nature of the structure. Reproduced with permission from Wang *et al.* (2003). Copyright (2003) by The American Physical Society.

and recorded. The entire pattern thus consists of many independent 'point' diffraction patterns (each for a slightly different incident beam direction) laid beside each other. Fig. 1.6.6.1 shows a CBED pattern from the wurtzite structure of ZnO, with the beam normal to the *c* axis (Wang *et al.*, 2003). The intensity variation along a line running through the centres of these discs (along the *c* axis) is not an even function, strongly violating Friedel's law for this elastic scattering. At higher scattering angles, curvature of the Ewald sphere allows three-dimensional symmetry elements to be determinated by taking account of 'out-of-zone' intensities in the outer higher-order Laue zone (HOLZ) rings near the edge of the detector. Since sub-ångstrom-diameter electron probes and nanometre X-ray laser probes (Spence *et al.*, 2012) are now being used, the effect of the inevitable coherent interference between overlapping convergent-beam orders on space-group determination must be considered (Spence & Zuo, 1992).

A systematic approach to space-group determination by CBED has been developed by several groups. In general, one would determine the symmetry of the projection diffraction group first (ignoring diffraction components along the beam direction *z*), then add the *z*-dependent information seen in HOLZ lines, allowing one to finally identify the point group from tables, by combining all this information. After indexing the pattern, in order to determine a unit cell the Bravais lattice is next determined. The form of the three-dimensional reciprocal lattice and its centring can usually be determined by noting the registry of Bragg spots in a HOLZ ring against those in the zero-order (ZOLZ) ring. Finally, by setting up certain special orientations, tests are applied for the presence of screw and glide elements, which are revealed by a characteristic dark line or cross within the CBED discs. Tables can again then be used to combine these translational symmetry elements with the previously determined point group, to find the space group. As a general experimental strategy, one first seeks mirror lines (perhaps seen in Kikuchi patterns), then follows these around using the two-axis goniometer fitted to modern TEM instruments in a systematic search for other symmetry elements. Reviews of the CBED method can be found in Steeds & Vincent (1983), in Goodman (1975), and in the texts by Tanaka *et al.* (1988). A textbook-level worked example of space-group determination by CBED can be found in Spence & Zuo (1992) and in the chapter by A. Eades in Williams & Carter (2009).

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1.7. Topics on space groups treated in Volumes A1 and E of *International Tables for Crystallography*

H. Wondratschek, U. Müller, D. B. Litvin and V. Kopský

1.7.1. Subgroups and supergroups of space groups

By H. Wondratschek

Relations between crystal structures play an important role for the comparison and classification of crystal structures, the analysis of phase transitions in the solid state, the understanding of topotactic reactions, and other applications. The relations can often be expressed by group–subgroup relations between the corresponding space groups. Such relations may be recognized from relations between the lattices and between the point groups[1] of the crystal structures.

In the first five editions of this Volume A of *International Tables for Crystallography*, subgroups and those supergroups of space groups that are space groups were listed for every space group. However, the listing was incomplete and it lacked additional information, such as, for example, possible unit-cell transformations and/or origin shifts involved. It became apparent that complete lists and more detailed data were necessary. Therefore, a supplementary volume of *International Tables for Crystallography* to this Volume A has been published: Volume A1, *Symmetry Relations between Space Groups* (2004; second edition 2010), abbreviated as *IT* A1 in this chapter. The listing of the subgroups and supergroups has thus been discontinued in this sixth edition of Volume A.

This chapter gives a short outline of the contents and applications of the relations listed in Volume A1. In addition, information on Volume E of *International Tables for Crystallography* is presented. Volume E lists the subperiodic groups, which are other kinds of subgroups of the space groups.

Volume A1 consists of three parts. Part 1 covers the theory of space groups and their subgroups, space-group relations between crystal structures and the corresponding Wyckoff positions, and the Bilbao Crystallographic Server (http://www.cryst.ehu.es/). This server is freely accessible and offers access to computer programs that display the subgroups and supergroups of the space groups and other relevant data. Part 2 of Volume A1 contains complete lists of the maximal subgroups of the plane groups and space groups, including unit-cell transformations and origin shifts, if applicable. An overview of the group–subgroup relations is also displayed in diagrams. Part 3 contains tables of relations between the Wyckoff positions of group–subgroup-related space groups and a guide to their use.

Example

The crystal structures of silicon, Si, and sphalerite, ZnS, belong to space-group types $Fd\bar{3}m$ (O_h^7; No. 227) and $F\bar{4}3m$ (T_d^2; No. 216) with lattice parameters $a_{Si} = 5.43$ Å and $a_{ZnS} = 5.41$ Å. The structure of sphalerite (zinc blende) is obtained from that of silicon by replacing alternately half of the Si atoms by Zn and half by S, and by adjusting the lattice parameter. This procedure is described in detail in Fig. 1.7.2.1. The strong connection between the two crystal structures is reflected in the relation between their space groups: the point group (crystal class) and the space group of sphalerite is a subgroup (of index 2) of that of silicon (ignoring the small difference in lattice parameters).

Data on subgroups and supergroups of the space groups are useful for the discussion of structural relations and phase transitions. It must be kept in mind, however, that group–subgroup relations only constitute symmetry relations. It is important, therefore, to ascertain that the consequential relations between the lattice parameters and between the atomic coordinates of the particles of the crystal structures also hold before a structural relation can be deduced from a symmetry relation.

Examples

NaCl and CaF_2 belong to the same space-group type, $Fm\bar{3}m$ (O_h^5; No. 225), and have lattice parameters $a_{NaCl} = 5.64$ Å and $a_{CaF_2} = 5.46$ Å. The ions, however, occupy unrelated positions and so the symmetry relation does not express a structural relation.

Pyrite, FeS_2, and solid carbon dioxide, CO_2, belong to the same space-group type, $Pa\bar{3}$ (T_h^6; No. 205). They have lattice parameters $a_{FeS_2} = 5.42$ Å and $a_{CO_2} = 5.55$ Å, and the particles occupy analogous Wyckoff positions. Nevertheless, the structures of these compounds are not related, because the positional parameters $x = 0.386$ of S in FeS_2 and $x = 0.118$ of O in CO_2 differ so much that the coordinations of the corresponding atoms are dissimilar.

To formulate group–subgroup relations some definitions are necessary. Subgroups and their distribution into conjugacy classes, normal subgroups, supergroups, maximal subgroups, minimal supergroups, proper subgroups, proper supergroups and index are defined for groups in general in Chapter 1.1. These definitions are used also for crystallographic groups like space groups. In the present chapter, the data of *IT* A1 are explained through many examples in order to enable the reader to use *IT* A1.

Examples

Maximal subgroups $\mathcal{H}$ of a space group $P1$ with basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are, among others, subgroups $P1$ for which $\mathbf{a}'' = p\mathbf{a}$, $\mathbf{b}'' = \mathbf{b}$, $\mathbf{c}'' = \mathbf{c}$, p prime. If p is not a prime number but a product of two integers $p = q \times r$, the subgroup $\mathcal{H}$ is not maximal because a proper subgroup $\mathcal{Z}$ of index q exists such that $\mathbf{a}' = q\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$. $\mathcal{Z}$ again has $\mathcal{H}$ as a proper subgroup of index r with $\mathcal{G} > \mathcal{Z} > \mathcal{H}$.

$P12_1/c1$ has maximal subgroups $P12_11$, $P1c1$ and $P\bar{1}$ with the same unit cell, whereas $P1$ is not a maximal subgroup of $P12_1/c1$: $P12_1/c1 > P12_11 > P1$; $P12_1/c1 > P1c1 > P1$; $P12_1/c1 > P\bar{1} > P1$. These are all possible chains of maximal subgroups for $P12_1/c1$ if the original translations are retained

[1] The point group determines both the symmetry of the physical properties of the macroscopic crystal and the symmetry of its ideal shape. Each space group belongs to a point group.

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completely. Correspondingly, the seven subgroups of index 4 with the same translations as the original space group $P6_3/mcm$ are obtained *via* the 21 different chains of Fig. 1.7.1.1.

While all group–subgroup relations considered here are relations between individual space groups, they are valid for all space groups of a space-group type, as the following example shows.

Example

A particular space group $P121$ has a subgroup $P1$ which is obtained from $P121$ by retaining all translations but eliminating all rotations and combinations of rotations with translations. For every space group of space-group type $P121$ such a subgroup $P1$ exists.

From this example it follows that the relationship exists, in an extended sense, for the two space-group types involved. One can, therefore, list these relationships by means of the symbols of the space-group types.

A three-dimensional space group may have subgroups with no translations (*i.e.* site-symmetry groups; *cf.* Section 1.4.5), or with one- or two-dimensional lattices of translations (*i.e.* line groups, frieze groups, rod groups, plane groups and layer groups), *cf.* Volume E of *International Tables for Crystallography*, or with a three-dimensional lattice of translations (space groups).

The number of subgroups of a space group is always infinite. Not only the number of all subgroups but even the number of all maximal subgroups of a given space group is infinite.

In this section, only those subgroups of a space group that are also space groups will be considered. All *maximal* subgroups of space groups are themselves space groups. To simplify the discussion, let us suppose that we know all maximal subgroups of a space group $\mathcal{G}$. In this case, *any* subgroup $\mathcal{H}$ of $\mathcal{G}$ may be obtained *via* a chain of maximal subgroups $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_{r-1}, \mathcal{H}_r$ such that $\mathcal{G}\ (=\mathcal{H}_0) > \mathcal{H}_1 > \mathcal{H}_2 > \ldots > \mathcal{H}_{r-1} > \mathcal{H}_r\ (=\mathcal{H})$, where $\mathcal{H}_j$ is a maximal subgroup of $\mathcal{H}_{j-1}$ of index $[i_j]$, with $j = 1, \ldots, r$. There may be many such chains between $\mathcal{G}$ and $\mathcal{H}$. On the other hand, all subgroups of $\mathcal{G}$ of a given index $[i]$ are obtained if all chains are constructed for which $[i_1] \times [i_2] \times \ldots \times [i_r] = [i]$ holds.

The index $[i]$ of a subgroup has a geometric significance. It determines the 'dilution' of symmetry operations of $\mathcal{H}$ compared with those of $\mathcal{G}$. The number of symmetry operations of $\mathcal{H}$ is $1/i$ times the number of symmetry operations of $\mathcal{G}$; since space groups are infinite groups, this is to be understood in the same way as 'the number of even numbers is one half of the number of all integer numbers'.

The infinite number of subgroups only occurs for a certain kind of subgroup and can be reduced as described below. It is thus useful to consider the different kinds of subgroups of a space group in the way introduced by Hermann (1929):

(1) By reducing the order of the point group, *i.e.* by eliminating all symmetry operations of some kind. The example $P12_11 \longrightarrow P1$ mentioned above is of this type;
(2) By loss of translations, *i.e.* by 'thinning out' the lattice of translations. For the space group $P121$ mentioned above this may happen in different ways:
   (*a*) by suppressing all translations of the kind $(2u+1)\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, where u, v and w are integers. The new basis is normally written $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$ and, hence, half of the twofold axes have been eliminated; or
   (*b*) by $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$, *i.e.* by thinning out the translations parallel to the twofold axes; or
   (*c*) again by $\mathbf{b}' = 2\mathbf{b}$ but replacing the twofold rotation axes by twofold screw axes.
(3) By combination of (1) and (2), *e.g.* by reducing the order of the point group and by thinning out the lattice of translations.

Subgroups of the first kind, (1), are called *translationengleiche* (or *t*-) subgroups because the set $\mathcal{T}$ of all (pure) translations is retained. In case (2), the point group $\mathcal{P}$ and thus the crystal class of the space group is unchanged. These subgroups are called *klassengleiche* or *k*-subgroups. In the general case (3), both the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ and the point group $\mathcal{P}$ are reduced; the subgroup has lost translations *and* belongs to a crystal class of lower order: these are *general* subgroups.

Obviously, the general subgroups are more difficult to survey than kinds (1) and (2). Fortunately, a theorem of Hermann (1929) states that if $\mathcal{H}$ is a proper subgroup of $\mathcal{G}$, then there always exists an intermediate group $\mathcal{M}$ such that $\mathcal{G} > \mathcal{M} > \mathcal{H}$, where $\mathcal{M}$ is a *t*-subgroup of $\mathcal{G}$ and $\mathcal{H}$ is a *k*-subgroup of $\mathcal{M}$. If $\mathcal{H} < \mathcal{G}$ is maximal, then either $\mathcal{M} = \mathcal{G}$ and $\mathcal{H}$ is a *k*-subgroup of $\mathcal{G}$ or $\mathcal{M} = \mathcal{H}$ and $\mathcal{H}$ is a *t*-subgroup of $\mathcal{G}$. It follows that a maximal subgroup of a space group $\mathcal{G}$ is either a *t*-subgroup or a *k*-subgroup of $\mathcal{G}$. According to this theorem, general subgroups can never occur among the maximal subgroups. They can, however, be derived by a stepwise process of linking maximal *t*-subgroups and maximal *k*-subgroups by the chains discussed above.

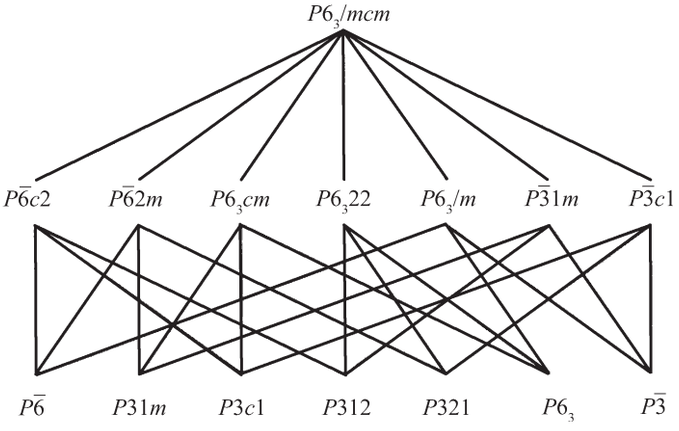

Figure 1.7.1.1
Space group $P6_3/mcm$ with *t*-subgroups of index 2 and 4. All 21 possible subgroup chains are displayed by lines.

1.7.1.1. *Translationengleiche* (or *t*-) subgroups of space groups

The 'point group' $\mathcal{P}$ of a given space group $\mathcal{G}$ is a finite group, *cf.* Chapter 1.3. Hence, the number of subgroups and consequently the number of maximal subgroups of $\mathcal{P}$ is finite. There exist, therefore, only a finite number of maximal *t*-subgroups of $\mathcal{G}$. The possible *t*-subgroups were first listed in *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, Band 1 (1935); corrections have been reported by Ascher *et al.* (1969). All maximal *t*-subgroups are listed individually for each space group $\mathcal{G}$ in *IT* A1 with the index, the (unconventional) Hermann–Mauguin symbol referred to the coordinate system of $\mathcal{G}$, the space-group number and conventional Hermann–Mauguin symbol, their general position and the transformation to the conventional coordinate system of $\mathcal{H}$. This may involve a change of basis and an origin shift from the coordinate system of $\mathcal{G}$.

1.7.1.2. *Klassengleiche* (or *k*-) subgroups of space groups

Every space group $\mathcal{G}$ has an infinite number of maximal *k*-subgroups. For dimensions 1, 2 and 3, however, it can be shown that the number of maximal *k*-subgroups is finite if subgroups belonging to the same affine space-group type as $\mathcal{G}$ are excluded. The number of maximal subgroups of $\mathcal{G}$ belonging to the same affine space-group type as $\mathcal{G}$ is always infinite; these subgroups are called maximal *isomorphic* subgroups. Maximal *non-isomorphic klassengleiche* subgroups of plane groups and space groups always have index 2, 3 or 4. They are listed individually in *IT* A1 together with the isomorphic subgroups of the same index. For practical reasons, the *k*-subgroups are distributed into two lists headed 'Loss of centring translations' and 'Enlarged (conventional) unit cell'. The data consist of the index of the subgroup $\mathcal{H}$, the lattice relation between the lattices of $\mathcal{H}$ and $\mathcal{G}$, the characterization of the space group $\mathcal{H}$, the general position of $\mathcal{H}$ and the transformation from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$.

1.7.1.3. Isomorphic subgroups of space groups

The existence of isomorphic subgroups is of special interest. There can be no proper isomorphic subgroups $\mathcal{H} < \mathcal{G}$ of finite groups $\mathcal{G}$ because the difference of the orders $|\mathcal{H}| < |\mathcal{G}|$ does not allow isomorphism. The point group $\mathcal{P}$ of a space group $\mathcal{G}$ is finite and its order cannot be reduced if $\mathcal{H}$ is to be isomorphic to $\mathcal{G}$. Therefore, isomorphic subgroups are necessarily *k*-subgroups.

The number of isomorphic maximal subgroups and thus the number of all isomorphic subgroups of any space group is infinite. It can be shown that maximal subgroups of space groups of index $i > 4$ are necessarily isomorphic. Depending on the crystallographic equivalence of the coordinate axes, the index of the subgroup is p, p^2 or p^3, where p is a prime. The isomorphic subgroups cannot be listed individually because of their number, but they can be listed as members of a few series. The series are mostly determined by the index p; the members may be normal subgroups of $\mathcal{G}$ or they form conjugacy classes the size of which is either p, p^2 or p^3. The individual members of a conjugacy class are determined by the locations of their origins. The size of the conjugacy class, a basis for the lattice of the subgroup, the generators of the individual isomorphic subgroups and the coordinate transformation from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$ are listed in *IT* A1 for all space-group types.

Examples

Isomorphic subgroups of $P1$: the space group $P1$ is an abelian space group, all of its subgroups are isomorphic and are normal subgroups. The index may be any prime p.

Isomorphic subgroups of $P\overline{1}$: the space group $P\overline{1}$ is not abelian and subgroups exist of types $P1$ and $P\overline{1}$. The latter are isomorphic. Those of index 2 are normal subgroups; for higher index $p > 2$ they form conjugacy classes of prime size p.

Enantiomorphic space groups have an infinite number of maximal isomorphic subgroups of the same type and an infinite number of maximal isomorphic subgroups of the enantiomorphic type.

Example

All *k*-subgroups $\mathcal{H}$ of a given space group $\mathcal{G} = P3_1$ with basis vectors $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = p\mathbf{c}$, where p is any prime number other than 3, are maximal isomorphic subgroups. They belong to space-group type $P3_1$ if $p = 1$ mod 3. They belong to the enantiomorphic space-group type $P3_2$ if $p = 2$ mod 3.

In principle there is no difference in importance between *t*-, non-isomorphic *k*- and isomorphic *k*-subgroups. Roughly speaking, a group–subgroup relation is 'strong' if the index [*i*] of the subgroup is low. All maximal *t*- and maximal non-isomorphic *k*-subgroups have indices less than four in $\mathbb{E}^2$ and less than five in $\mathbb{E}^3$, index four already being rather exceptional. Maximal isomorphic *k*-subgroups of arbitrarily high index exist for every space group.

1.7.1.4. Supergroups

Sometimes a space group $\mathcal{H}$ is known and the possible space groups $\mathcal{G}$, of which $\mathcal{H}$ is a subgroup, are of interest. A space group $\mathcal{R}$ is called a *minimal supergroup* of a space group $\mathcal{G}$ if $\mathcal{G}$ is a maximal subgroup of $\mathcal{R}$.

Examples of minimal supergroups

In Fig. 1.7.1.1, the space group $P6_3/mcm$ is a minimal supergroup of $P\overline{6}c2$, ..., $P\overline{3}c1$; $P\overline{6}c2$ is a minimal supergroup of $P\overline{6}$, $P3c1$ and $P312$; *etc*.

If $\mathcal{G}$ is a maximal *t*-subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal *t*-supergroup of $\mathcal{G}$. If $\mathcal{G}$ is a maximal *k*-subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal *k*-supergroup of $\mathcal{G}$. Finally, if $\mathcal{G}$ is a maximal isomorphic subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal isomorphic supergroup of $\mathcal{G}$. Data for minimal *t*- and minimal non-isomorphic *k*-supergroups are listed in *IT* A1, although in a less explicit way than that in which the subgroups are listed. The data essentially make the detailed subgroup data usable for the search for supergroups of space groups. Data on minimal isomorphic supergroups are not listed because they can be derived from the corresponding subgroup relations.

The search for supergroups $\mathcal{R} > \mathcal{G}$ of a space group $\mathcal{G}$ differs from the search for subgroups $\mathcal{H} < \mathcal{G}$ in one essential point: when looking for subgroups one knows the available group elements, namely the elements $g \in \mathcal{G}$; when looking for supergroups, any isometry $f \in \mathcal{E}$ may be a possible element of $\mathcal{R}$, $f \in \mathcal{R}$, where $\mathcal{E}$ is the Euclidean group of all isometries.

As we are mainly interested in the symmetries of crystal structures, it is reasonable only to look for groups $\mathcal{R}$ that are themselves space groups. In this way the search for supergroups of space groups is a reversal of the search for subgroups. Nevertheless, even then there are new phenomena; only two of these shall be mentioned here.

Example

For a given space group $P\overline{1}$, there is only one *t*-subgroup $P1$. However, for a space group $P1$, there is a continuously infinite number of *t*-supergroups $P\overline{1}$. Referred to the unit cell of $P1$, an additional centre of inversion can be placed in the range $0 \le x < \frac{1}{2}$, $0 \le y < \frac{1}{2}$, $0 \le z < \frac{1}{2}$. The centre in each of these locations leads to a new supergroup resulting in a continuous set of *t*-supergroups.

If $\mathcal{R}$ is a *t*-supergroup of $\mathcal{G}$ belonging to a crystal system with higher symmetry than that of $\mathcal{G}$, then the metric of $\mathcal{G}$ has to fulfil the conditions of the metric of $\mathcal{R}$. For example, if a tetragonal space group $\mathcal{G}$ has a cubic *t*-supergroup $\mathcal{R}$, then the lattice of $\mathcal{G}$ also has to have cubic symmetry.

In practice, small differences in the lattice parameters of $\mathcal{G}$ and $\mathcal{R}$ will occur, because lattice deviations can accompany a structural relationship.

1.7.2. Relations between Wyckoff positions for group–subgroup-related space groups

By U. Müller

1.7.2.1. Symmetry relations between crystal structures

The crystal structures of two compounds are *isotypic* if their atoms are arranged in the same way and if they have the same or the enantiomorphic space group. The absolute values of the lattice parameters and interatomic distances may differ and small deviations are permitted for non-fixed coordinates of corresponding atoms. The axial ratios and interaxial angles must be similar. Two structures are *homeotypic* if the conditions for isotypism are relaxed because (Lima-de-Faria *et al.*, 1990): (1) their space groups differ, allowing for a group–subgroup relation; (2) the geometric conditions differ (axial ratios, interaxial angles, atomic coordinates); or (3) an atomic position in one structure is occupied in an ordered way by various atomic species in the other structure (substitution derivatives or after a misorder–order phase transition).[2]

Group–subgroup relations between the space groups of homeotypic crystal structures are particularly suited to disclosing the relationship. A standardized procedure to set forth such relations was developed by Bärnighausen (1980). The concept is to start from a simple, highly symmetrical crystal structure and to derive more complicated structures by distortions and/or substitutions of atoms. A tree of group–subgroup relations between the space groups involved, now called a *Bärnighausen tree*, serves as the main guideline. The highly symmetrical starting structure is called the *aristotype* after Megaw (1973) or *basic structure* after Buerger (1947, 1951) or, in the literature on phase transitions in physics, *prototype* or *parent structure*. The derived structures are the *hettotypes* or *derivative structures* or, in phase-transition physics, *distorted structures* or *daughter phases*. In Megaw's terminology, the structures mentioned in the tree form a *family of structures*.

Detailed instructions on how to form a Bärnighausen tree, the information that can be drawn from it and some possible pitfalls are given in the second edition of *IT* A1, Chapter 1.6 and in the book by Müller (2013). In any case, setting up group–subgroup relations requires a thorough monitoring of how the Wyckoff positions develop from a group to a subgroup for every position occupied. The following examples give a concise impression of such relations.

1.7.2.2. Substitution derivatives

As an example, Fig. 1.7.2.1 shows the simple relation between diamond and zinc blende. This is an example of a substitution derivative. The reduction of the space-group symmetry from diamond to zinc blende is depicted by an arrow which points from the higher-symmetry space group of diamond to the lower-symmetry space group of zinc blende. The subgroup is *translationengleiche* of index 2, marked by *t*2 in the middle of the arrow. *Translationengleiche* means that the subgroup has the same translational lattice (the same size and dimensions of the primitive unit cell) but its crystal class is of reduced symmetry. The index [*i*] is the factor by which the total number of symmetry operations has been reduced, *i.e.* the subgroup has 1/*i* as many symmetry operations; as mentioned in Section 1.7.1, this is to be understood in the same way as 'the number of even numbers is half as many as the number of all integer numbers'.

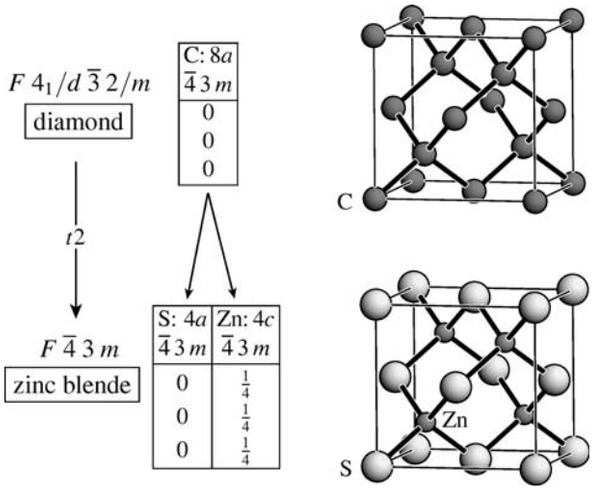

Figure 1.7.2.1
Group–subgroup relation from the aristotype diamond to its hettotype zinc blende. The numerical values in the boxes are atomic coordinates.

The consequences of the symmetry reduction on the positions occupied by the atoms are important. As shown in the boxes next to the space-group symbols in Fig. 1.7.2.1, the carbon atoms in diamond occupy the Wyckoff position 8*a* of the space group $F\,4_1/d\,\bar{3}\,2/m$. Upon transition to zinc blende, this position splits into two independent Wyckoff positions, 4*a* and 4*c*, of the subgroup $F\,\bar{4}\,3\,m$, rendering possible occupation by atoms of the two different species zinc and sulfur. The site symmetry $\bar{4}3m$ remains unchanged for all atoms.

Further substitutions of atoms require additional symmetry reductions. For example, in chalcopyrite, $CuFeS_2$, the zinc atoms of zinc blende have been substituted by copper and iron atoms. This implies a symmetry reduction from $F\bar{4}3m$ to its subgroup $I\bar{4}2d$; this requires one *translationengleiche* and two steps of *klassengleiche* group–subgroup relations, including a doubling of the unit cell.

1.7.2.3. Phase transitions

Fig. 1.7.2.2 shows derivatives of the cubic ReO_3 structure type that result from distortions of this high-symmetry structure. WO_3 itself does not adopt this structure, only several distorted variants. The first step of symmetry reduction involves a tetragonal distortion of the cubic ReO_3 structure resulting in the space group *P*4/*mmm*; no example with this symmetry is yet known. The second step leads to a *klassengleiche* subgroup of index 2 (marked *k*2 in the arrow), resulting in the structure of high-temperature WO_3, which is the most symmetrical known modification of WO_3. *Klassengleiche* means that the subgroup belongs to the same crystal class, but it has lost translational symmetry (its primitive unit cell has been enlarged). In this case this is a doubling of the size of the unit cell ($\mathbf{a}-\mathbf{b}, \mathbf{a}+\mathbf{b}, \mathbf{c}$) combined with an origin shift of $-\frac{1}{2}, 0, 0$ (in the coordinate system of *P*4/*mmm*). This cell transformation and origin shift cause a change of the atomic coordinates of the metal atom from 0, 0, 0 to $\frac{1}{4}, \frac{1}{4}, \sim 0.0$ (the

[2] In the strict sense, two isotypic compounds do not have the same space group if their translation lattices (lattice dimensions) differ. However, such a strict treatment would render it impossible to apply group-theoretical methods in crystal chemistry and crystal physics. Therefore, we treat isotypic and homeotypic structures as if their translation lattices were the same or related by an integral enlargement factor. For more details see the second edition of *IT* A1 (2010), Sections 1.2.7 and 1.6.4.1. We prefer the term 'misorder' instead of the usual 'disorder' because there still is order in the 'disordered' structure, although it is a reduced order.

decimal value indicates that the coordinate is not fixed by symmetry). Simultaneously, the site symmetry of the metal atom is reduced from 4/*mmm* to 4*mm* and the z coordinate becomes independent. In fact, the W atom is shifted from $z = 0$ to $z = 0.066$, *i.e.* it is not situated in the centre of the octahedron of the surrounding O atoms. This shift is the cause of the symmetry reduction. There is no splitting of the Wyckoff positions in this step of symmetry reduction, but a decrease of the site symmetries of all atoms.

When cooled, at 1170 K *HT*-WO_3 is transformed to α-WO_3. This involves mutual rotations of the coordination octahedra along **c** and requires another step of symmetry reduction. Again, the Wyckoff positions do not split in this step of symmetry reduction, but the site symmetries of all atoms are further decreased.

Upon further cooling, WO_3 undergoes several other phase transitions that involve additional distortions and, in each case, an additional symmetry reduction to another subgroup (not shown in Fig. 1.7.2.2). For more details see Müller (2013), Section 11.6, and references therein.

1.7.2.4. Domain structures

In the case of phase transitions and of topotactic reactions[3] that involve a symmetry reduction, the kind of group–subgroup relation determines how many kinds of domains and what domain states can be formed. If the lower-symmetry product results from a *translationengleiche* group–subgroup relation, twinned crystals are to be expected. A *klassengleiche* group–subgroup relation will cause antiphase domains. The number of different kinds of twin or antiphase domains corresponds to the index of the symmetry reduction. For example, the phase transition from *HT*-WO_3 to α-WO_3 involves a *klassengleiche* group–subgroup relation of index 2 (*k*2 in Fig. 1.7.2.2); no twins will be formed, but two kinds of antiphase domains can be expected.

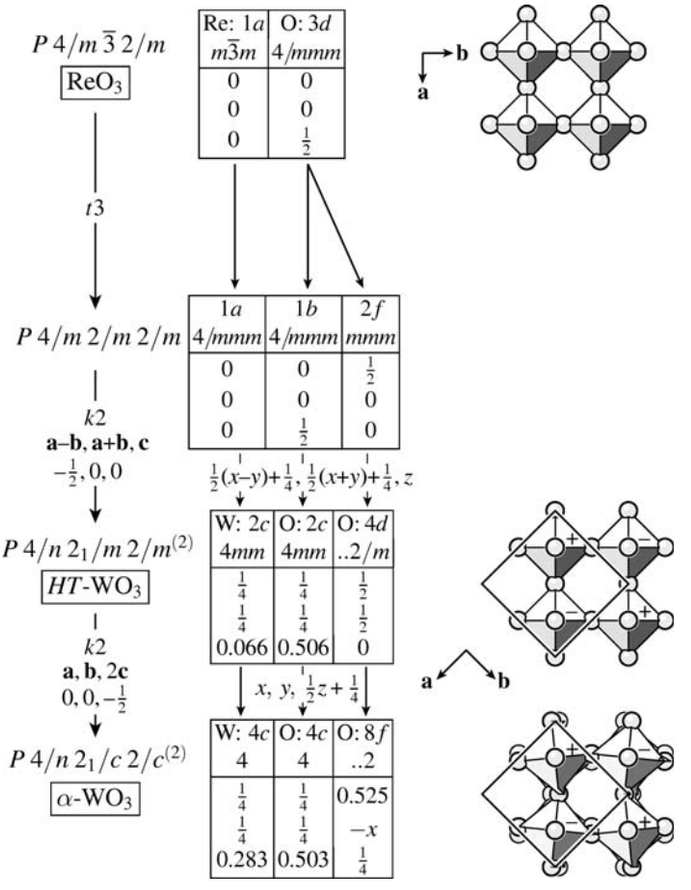

Figure 1.7.2.2
Group–subgroup relations (Bärnighausen tree) from the ReO_3 type to two polymorphic forms of WO_3. The superscript (2) after the space-group symbols states the origin choice. + and − in the images of high-temperature WO_3 and α-WO_3 indicate the direction of the z shifts of the W atoms from the octahedron centres. Structural data for WO_3 are taken from Locherer *et al.* (1999).

1.7.2.5. Presentation of the relations between the Wyckoff positions among group–subgroup-related space groups

Group–subgroup relations as outlined in the preceding sections can only be correct if all atomic positions of the hettotypes result directly from those of the aristotype.

Every group–subgroup relation between space groups entails specific relations between their Wyckoff positions. If the index of symmetry reduction is 2, a Wyckoff position either splits into two symmetry-independent positions that keep the site symmetry, or there is no splitting and the site symmetry is reduced. If the index is 3 or higher, a Wyckoff position either splits, or its site symmetry is reduced, or both happen. Given the relative settings and origin choices of a space group and its subgroup, there exist unique relations between their Wyckoff positions. Laws governing these relations are considered in Chapter 1.5 of the second edition of *IT* A1.

Volume A1, Part 3, *Relations between the Wyckoff positions*, contains tables for all space groups. For every one of them, all maximal subgroups are listed, including the corresponding coordinate transformations. For all Wyckoff positions of a space group the relations to the Wyckoff positions of the subgroups are given. This includes the infinitely many maximal isomorphic subgroups, for which general formulae are given. Isomorphic subgroups are a special kind of *klassengleiche* subgroup that belong to the same or the enantiomorphic space-group type, *i.e.* group and subgroup have the same or the enantiomorphic space-group symbol; the unit cell of the subgroup is increased by some integral factor, which is p, p^2 or p^3 (p = prime number) in the case of maximal isomorphic subgroups.

[3] A topotactic reaction is a chemical reaction in the solid state where the orientation of the product crystal is determined by the orientation of the educt crystal.

1.7.3. Relationships between space groups and subperiodic groups

By D. B. Litvin and V. Kopský

The present volume in the series *International Tables for Crystallography* (Volume A: *Space-Group Symmetry*) treats one-, two- and three-dimensional space groups. Volume E in the series, *Subperiodic Groups* (2010), treats two- and three-dimensional subperiodic groups: frieze groups (groups in two-dimensional space with translations in a one-dimensional subspace), rod groups (groups in three-dimensional space with translations in a one-dimensional subspace) and layer groups (groups in three-dimensional space with translations in a two-dimensional subspace). In the same way in which three-dimensional space groups are used to classify the atomic structure of three-dimensional crystals, the subperiodic groups are used to classify the atomic structure of other crystalline structures, such as liquid crystals, domain interfaces, twins and thin films.

Orientation orbit ($hkil$)	Conventional basis of the scanning group $\mathbf{a}'$ $\mathbf{b}'$ $\mathbf{d}$	Scanning group $\mathcal{H}$	Linear orbit $s\mathbf{d}$	Sectional layer group $\mathcal{L}(s\mathbf{d})$
(0001)	**a** **b** **c**	$P\bar{3}m1$	$0\mathbf{d}$, $\frac{1}{2}\mathbf{d}$	$p\bar{3}m1$ L72
			$[s\mathbf{d}, -s\mathbf{d}]$	$p3m1$ L69

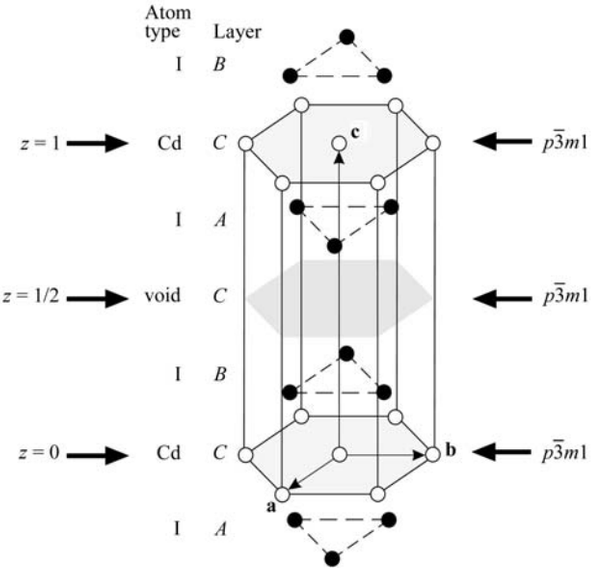

Figure 1.7.3.1
The scanning table for the space-group type $P\bar{3}m1$ (164) and orientation orbit (0001), and the structure of cadmium iodide, CdI_2. Cadmium and iodine ions are denoted by open and filled circles, respectively.

In Volume A, the relationship between the space group of a crystal and the point-group symmetry of individual points in the crystal is given by site symmetries, the point-group subgroups of the space group that leave the points invariant. In Volume E, an analogous relationship is given between the space group of a crystal and the subperiodic-group symmetry of planes that transect the crystal. Volume E contains *scanning tables* (with supplementary tables in Kopský & Litvin, 2004) from which the layer-group subgroups of the space group (called *sectional layer groups*) that leave the transecting planes invariant can be determined. The first attempts to derive sectional layer groups were made by Wondratschek (1971) and by using software written by Guigas (1971). Davies & Dirl (1993*a*,*b*) developed software for finding subgroups of space groups which was modified to find sectional layer groups. The use and determination of sectional layer groups have also been discussed by Janovec *et al.* (1988), Kopský & Litvin (1989) and Fuksa *et al.* (1993).

In Fig. 1.7.3.1, part of the scanning table for the space group $P\bar{3}m1$ (164) is given. From this one can determine the layer-group subgroups of $P\bar{3}m1$ that are symmetries of planes of orientation ($hkil$) = (0001). Vectors $\mathbf{a}'$ and $\mathbf{b}'$ are basic vectors of the translational subgroup of the layer-group symmetry of planes of this orientation. The vector **d** defines the *scanning direction* and is used to define the position of the plane within the crystal. The *linear orbit* is the set of all parallel planes obtained by applying all elements of the space group to any one plane. The *sectional layer group* is the layer subgroup of the space group that leaves the plane invariant.

Sectional layer groups were introduced by Holser (1958*a*,*b*) in connection with the consideration of domain walls and twin boundaries as symmetry groups of planes bisecting a crystal. The mutual orientation of the two domains separated by a domain wall or twin boundary is not arbitrary, but has crystallographic restrictions. The group-theoretical basis for an analysis of domain pairs is given by Janovec (1972), and the structure of domain walls and twin boundaries is considered by Janovec (1981) and Zikmund (1984) [see also Janovec & Přívratská (2014)].

Layer symmetries have been used in *bicrystallography*. The term *bicrystal* was introduced by Pond & Bollmann (1979) in the study of grain boundaries [see also Pond & Vlachavas (1983) and Vlachavas (1985)]. A bicrystal is in general an edifice where two crystals, usually of the same structure but of different, possibly arbitrary, orientations, meet at a common boundary. The sectional layer groups describe the symmetries of such a boundary [see Volume E (2010), Section 5.2.5.2].

An example of the application of the scanning tables to determine the layer-group symmetry of planes in a crystal is given in Section 1.7.3.1. In Section 1.7.3.2 the derivation of the layer-group symmetry of a domain wall is described.

1.7.3.1. Layer symmetries in three-dimensional crystal structures

Fig. 1.7.3.1 shows the crystal structure of cadmium iodide, CdI_2. The space group of this crystal is of type $P\bar{3}m1$ (164). The anions form a hexagonal close packing of spheres and the cations occupy half of the octahedral holes, filling one of the alternate layers. In close-packing notation, the CdI_2 structure is

A	*C*	*B*	*C*
I	Cd	I	void

From the scanning tables, we obtain for planes with the (0001) orientation and at heights $z = 0$ or $z = \frac{1}{2}$ a sectional layer-group symmetry type $p\bar{3}m1$ (layer group No. 72, or L72 for short), and for planes of this orientation at any other height a sectional layer-group symmetry type $p3m1$ (L69).

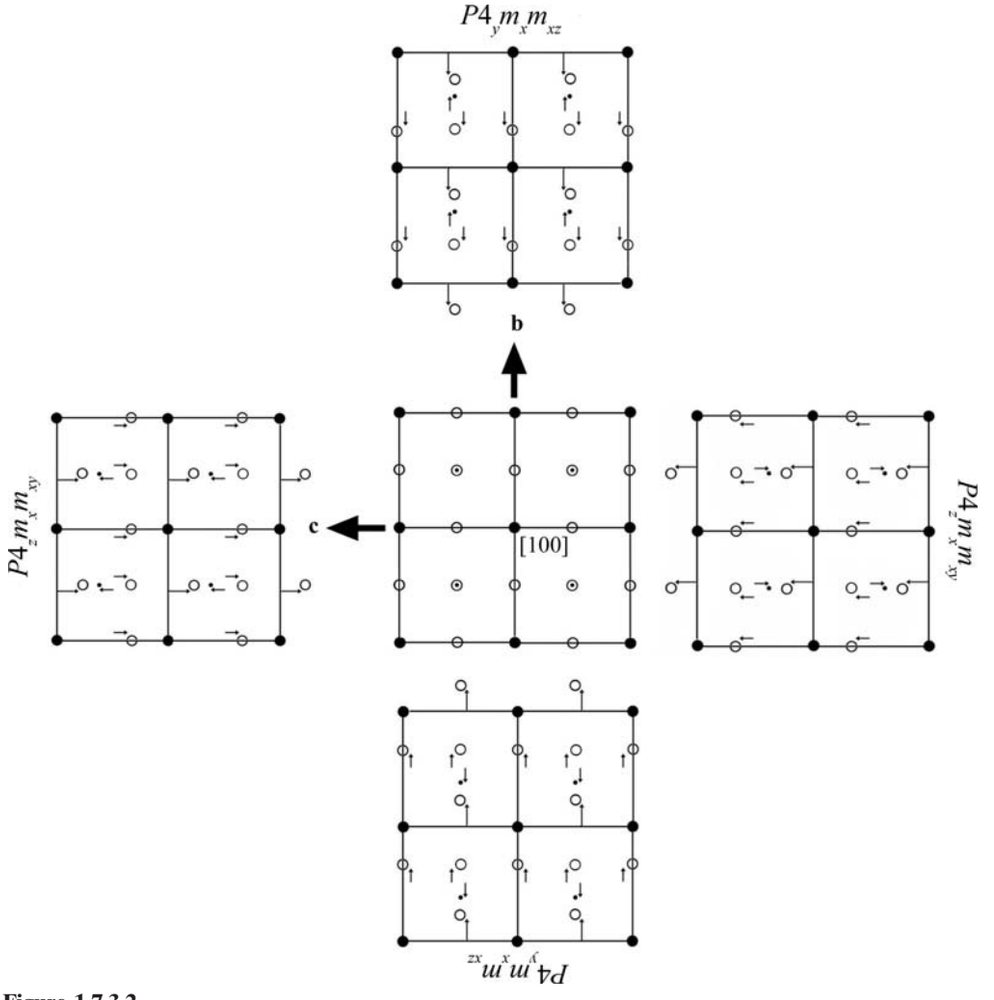

Figure 1.7.3.2
At the centre is the structure of the cubic phase of barium titanate, $BaTiO_3$, of symmetry type $Pm\bar{3}m$, surrounded by the structures of four of the six single-domain states of the tetragonal phase of symmetry type $P4mm$. All the diagrams are projections along the [100] direction. Arrows depict the atomic displacement amplitudes from their cubic-phase positions.

The $x, y, 0$ plane contains cadmium ions. This plane is a constituent of the orbit of planes of orientation (0001) passing through the points with coordinates 0, 0, u, where u is an integer. All these planes contain cadmium ions in the same arrangement (C layer filled with Cd).

The plane at height $z = \frac{1}{2}$ is a constituent of the orbit of planes of orientation (0001) passing through the points with coordinates 0, 0, $u + \frac{1}{2}$. All these planes contain only voids and lie midway between A and B layers of iodine ions with the B layer below and the A layer above the plane.

The planes at levels $z = \frac{1}{4}$ and $z = \frac{3}{4}$ contain B and A layers of iodine ions, respectively. These planes and all planes related to them by translations $t(0, 0, u)$ belong to the same orbit because the operations $\bar{3}$ exchange the A and B layers.

1.7.3.2. The symmetry of domain walls

The cubic phase of barium titanate $BaTiO_3$, of symmetry type $Pm\bar{3}m$, undergoes a phase transition to a tetragonal phase of symmetry type $P4mm$ which can give rise to six distinct single-domain states (Janovec *et al.*, 2004). This is represented in Fig. 1.7.3.2, where at the centre are four unit cells of the cubic phase with barium and titanium atoms represented by large and small filled circles, respectively, and oxygen atoms, which are located at the centre of each unit-cell face, as open circles. A cubic-to-tetragonal phase transition gives rise to atomic displacements represented by arrows, and to six single-domain states, four of which are depicted in the figure. The polar tetragonal symmetry of each of these tetragonal domain states is also shown.

In determining the symmetry of a domain wall, we first construct a *domain twin* (Janovec & Přívratská, 2014): we choose two single-domain states, for this example the two in Fig. 1.7.3.2 with symmetry $P4_zm_xm_{xy}$, and construct a *domain pair* consisting of the superposition of these two single-domain states, see Fig. 1.7.3.3. The domain twin we choose to construct is obtained by passing a plane of orientation (010) through this domain pair at the origin and deleting from one side of the plane the atoms of one of the single-domain states, and the atoms of the second single-domain state from the other side of the plane, see Fig. 1.7.3.4. The plane is referred to as the *central plane of the domain wall*, and the atoms in and near this plane as the *domain wall*.

The symmetry of the central plane of the domain wall is determined from the symmetry of the domain pair and the scanning tables: The symmetry of the domain pair is the group of operations that either leaves both single-domain states invariant or simultaneously switches the two domain states. $P4_zm_xm_{xy}$ leaves both single-domain states invariant and the symmetry operation of spatial inversion switches the two single-domain states, see Fig. 1.7.3.3. Consequently, the domain-pair symmetry is $P4_z/m_zm_xm_{xy} = P4_zm_xm_{xy} \cup \{\bar{1}|0\}P4_zm_xm_{xy}$. The symmetry of the central plane is determined from the scanning table for the space group $P4_z/m_zm_xm_{xy}$, the orientation orbit (010), the orientation of the domain wall and the linear orbit 0**d**, since the central plane of the

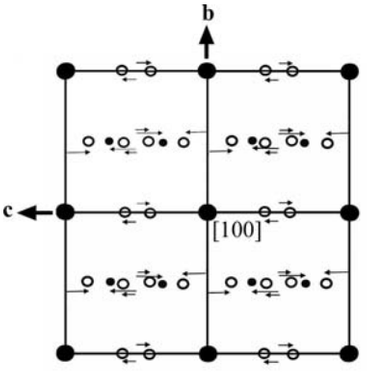

Figure 1.7.3.3
The *domain pair* of symmetry $P4_z/m_zm_xm_{xy}$ consisting of the superposition of those two single-domain states of tetragonal symmetry $P4_zm_xm_{xy}$ shown in Fig. 1.7.3.2. The diagram is a projection along the [100] direction.

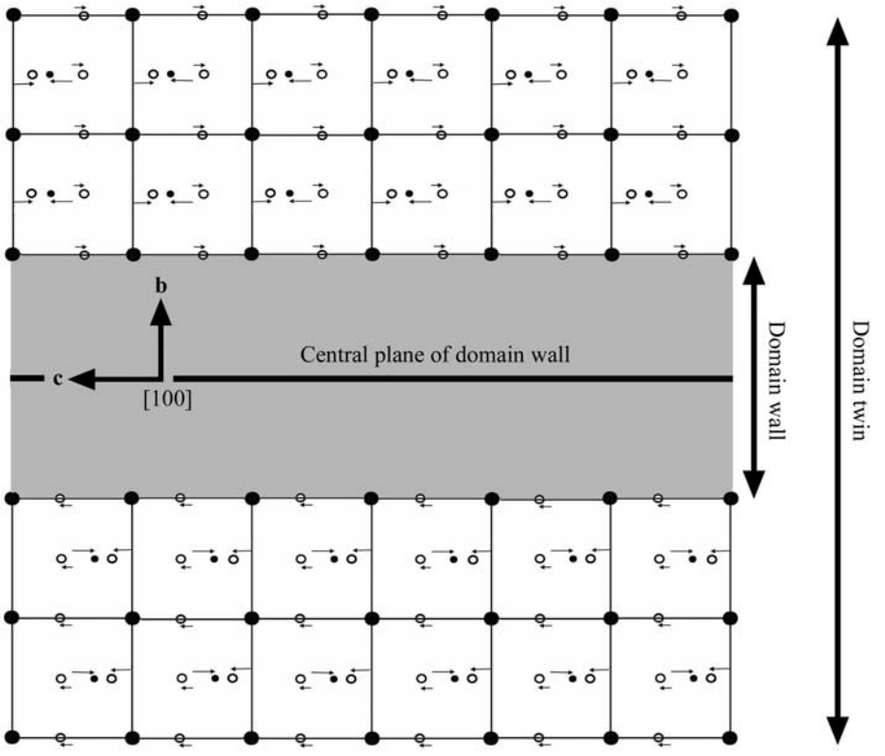

Figure 1.7.3.4
The domain twin consisting of the two domain states of tetragonal symmetry $P4_zm_xm_{xy}$ and a domain wall of orientation (010) passing through the origin of the domain twin.

wall passes through the origin (Volume E, 2010). The symmetry of the central plane is the sectional layer group $pm_xm_zm_y$, where p denotes the lattice of translations in the x, 0, z plane.

Let **n** denote a unit vector perpendicular to the central plane of the domain wall; in this example **n** is in the [010] direction. The symmetry of the domain wall consists of:

(1) all elements of the symmetry group of the central plane that leave **n** and both domain states invariant, *i.e.* in this example, all translations of p, 1 and m_x; and

(2) all elements of the symmetry group of the central plane that invert **n** and switch the domain states, *i.e.* in this example, 2_x and $\overline{1}$.

The symmetry of the domain wall is then $p2_x/m_x$.

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2.1. Guide to the use of the space-group tables

Th. Hahn, A. Looijenga-Vos, M. I. Aroyo, H. D. Flack, K. Momma and P. Konstantinov

In this part of the volume, tables and diagrams of crystallographic data for the 17 types of plane groups (Chapter 2.2) and the 230 types of space groups (Chapter 2.3) are presented. With the exception of the data for maximal subgroups and minimal supergroups (which have been transferred to Volume A1), the crystallographic data presented in Chapters 2.2 and 2.3 closely follow those in the fifth (2002) edition of Volume A, hereafter *IT* A (2002). This chapter is a guide to understanding and using these data.

Only a minimum of theory is provided here, as the emphasis is on the practical use of the data. For the theoretical background to these data, the reader is referred to Parts 1 and 3, which also include suitable references. A textbook explaining space-group symmetry and the use of the data in Chapters 2.2 and 2.3 (with exercises) is provided by Hahn & Wondratschek (1994); see also Müller (2013).

Section 2.1.1 displays, with the help of an extensive synoptic table, the classification of the 17 plane groups and 230 space groups. This is followed by an explanation of the characterization of the conventional crystallographic coordinate systems, including the symbols for the centring types of lattices and cells. Section 2.1.2 lists the alphanumeric and graphical symbols for symmetry elements and symmetry operations used throughout this volume. The lists are accompanied by notes and cross-references to related IUCr nomenclature reports. Section 2.1.3 explains in a systematic fashion, with many examples and figures, all the entries and diagrams in the order in which they occur in the plane-group and space-group tables of Chapters 2.2 and 2.3. Detailed treatments are given for the Hermann–Mauguin space-group symbols, the space-group diagrams, the general and special positions, the reflections conditions, monoclinic space groups, and the two crystallographic space groups in one dimension (which are also known as the line groups and are treated in Section 2.1.3.16). Section 2.1.4 discusses the computer generation of the space-group tables in this and earlier editions of the volume.

2.1.1. Conventional descriptions of plane and space groups

By Th. Hahn and A. Looijenga-Vos

2.1.1.1. Classification of space groups

In this volume, the plane groups and space groups are classified according to three criteria:

(i) According to *geometric crystal classes*, *i.e.* according to the crystallographic point group to which a particular space group belongs. There are 10 crystal classes in two dimensions and 32 in three dimensions. They are described and listed in Chapter 3.2 and in column 4 of Table 2.1.1.1. [For arithmetic crystal classes, see Chapter 1.3 and Table 2.1.3.3 in this volume, and Chapter 1.4 of *International Tables for Crystallography*, Vol. C (2004).]

(ii) According to *crystal families*. The term crystal family designates the classification of the 17 plane groups into four categories and of the 230 space groups into *six* categories, as displayed in column 1 of Table 2.1.1.1. Here all 'hexagonal', 'trigonal' and 'rhombohedral' space groups are contained in one family, the hexagonal crystal family. The 'crystal family' thus corresponds to the term 'crystal system', as used frequently in the American and Russian literature.

The crystal families are symbolized by the lower-case letters *a*, *m*, *o*, *t*, *h*, *c*, as listed in column 2 of Table 2.1.1.1. If these letters are combined with the appropriate capital letters for the lattice-centring types (*cf.* Table 2.1.1.2), symbols for the 14 Bravais lattices result. These symbols and their occurrence in the crystal families are shown in column 8 of Table 2.1.1.1; *mS* and *oS* are the standard setting-independent symbols for the centred monoclinic and the one-face-centred orthorhombic Bravais lattices, *cf.* de Wolff *et al.* (1985); symbols between parentheses represent alternative settings of these Bravais lattices.

(iii) According to *crystal systems*. This classification collects the plane groups into four categories and the space groups into *seven* categories. The classifications according to crystal families and crystal systems are the same for two dimensions.

For three dimensions, this applies to the triclinic, monoclinic, orthorhombic, tetragonal and cubic systems. The only complication exists in the hexagonal crystal family, for which several subdivisions into systems have been proposed in the literature. In this volume [as well as in *International Tables for X-ray Crystallography* (1952), hereafter *IT* (1952), and the subsequent editions of *IT*], the space groups of the hexagonal crystal family are grouped into two 'crystal systems' as follows: all space groups belonging to the five crystal classes 3, $\bar{3}$, 32, 3*m* and $\bar{3}m$, *i.e.* having 3, 3_1, 3_2 or $\bar{3}$ as principal axis, form the *trigonal* crystal system, irrespective of whether the Bravais lattice is *hP* or *hR*; all space groups belonging to the seven crystal classes 6, $\bar{6}$, 6/*m*, 622, 6*mm*, $\bar{6}2m$ and 6/*mmm*, *i.e.* having 6, 6_1, 6_2, 6_3, 6_4, 6_5 or $\bar{6}$ as principal axis, form the *hexagonal* crystal system; here the lattice is always *hP* (*cf.* Chapter 1.3). The crystal systems, as defined above, are listed in column 3 of Table 2.1.1.1.

A different subdivision of the hexagonal crystal family is in use, mainly in the French literature. It consists of grouping all space groups based on the hexagonal Bravais lattice *hP* (lattice point symmetry 6/*mmm*) into the 'hexagonal' system and all space groups based on the rhombohedral Bravais lattice *hR* (lattice point symmetry $\bar{3}m$) into the 'rhombohedral' system. In Chapter 1.3, these systems are called 'lattice systems'. They were called 'Bravais systems' in earlier editions of this volume.

The theoretical background for the classification of space groups is provided in Chapter 1.3.

2.1.1.2. Conventional coordinate systems and cells

A plane group or space group usually is described by means of a *crystallographic coordinate system*, consisting of a *crystallographic basis* (basis vectors are lattice vectors) and a *crystallographic origin* (origin at a centre of symmetry or at

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Table 2.1.1.1
Crystal families, crystal systems, conventional coordinate systems and Bravais lattices in one, two and three dimensions

Crystal family	Symbol†	Crystal system	Crystallographic point groups‡	No. of space groups	Conventional coordinate system		Bravais lattices†
					Restrictions on cell parameters	Parameters to be determined	
One dimension							
–	–	–	1, $\boxed{m}$	2	None	a	$\not\!p$
Two dimensions							
Oblique (monoclinic)	m	Oblique	1, $\boxed{2}$	2	None	a, b γ§	mp
Rectangular (orthorhombic)	o	Rectangular	m, $\boxed{2mm}$	7	$\gamma = 90°$	a, b	op oc
Square (tetragonal)	t	Square	$\boxed{4}$, $\boxed{4mm}$	3	$a = b$ $\gamma = 90°$	a	tp
Hexagonal	h	Hexagonal	3, $\boxed{6}$ $3m$, $\boxed{6mm}$	5	$a = b$ $\gamma = 120°$	a	hp
Three dimensions							
Triclinic (anorthic)	a	Triclinic	1, $\boxed{\bar{1}}$	2	None	a, b, c α, β, γ	aP
Monoclinic	m	Monoclinic	$2, m$, $\boxed{2/m}$	13	b-unique setting $\alpha = \gamma = 90°$	a, b, c β §	mP mS¶ (mC, mA, mI)
					c-unique setting $\alpha = \beta = 90°$	a, b, c γ §	mP mS¶ (mA, mB, mI)
Orthorhombic	o	Orthorhombic	222, $mm2$, $\boxed{mmm}$	59	$\alpha = \beta = \gamma = 90°$	a, b, c	oP oS¶ (oC, oA, oB) oI oF
Tetragonal	t	Tetragonal	$4, \bar{4}$, $\boxed{4/m}$ $422, 4mm, \bar{4}2m$, $\boxed{4/mmm}$	68	$a = b$ $\alpha = \beta = \gamma = 90°$	a, c	tP tI
Hexagonal	h	Trigonal	3, $\boxed{\bar{3}}$ $32, 3m$, $\boxed{\bar{3}m}$	18	$a = b$ $\alpha = \beta = 90°$, $\gamma = 120°$	a, c	hP
				7	$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell) $a = b$ $\alpha = \beta = 90°, \gamma = 120°$ (hexagonal axes, triple obverse cell)	a, α	hR
		Hexagonal	$6, \bar{6}$, $\boxed{6/m}$ $622, \bar{6}mm, \bar{6}2m$, $\boxed{6/mmm}$	27	$a = b$ $\alpha = \beta = 90°, \gamma = 120°$	a, c	hP
Cubic	c	Cubic	23, $\boxed{m\bar{3}}$ $432, \bar{4}3m$, $\boxed{m\bar{3}m}$	36	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	cP cI cF

† The symbols for crystal families (column 2) and Bravais lattices (column 8) were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).
‡ Symbols surrounded by dashed or full lines indicate Laue groups; full lines indicate Laue groups which are also lattice point symmetries (holohedries).
§ These angles are conventionally taken to be non-acute, *i.e.* $\geq 90°$.
¶ For the use of the letter *S* as a new general, setting-independent 'centring symbol' for monoclinic and orthorhombic Bravais lattices, see de Wolff *et al.* (1985).

a point of high site symmetry). The choice of such a coordinate system is not mandatory, since in principle a crystal structure can be referred to any coordinate system; *cf.* Chapters 1.3 and 1.5.

The selection of a crystallographic coordinate system is not unique. Conventionally, a right-handed set of basis vectors is taken such that the symmetry of the plane or space group is displayed best. With this convention, which is followed in the present volume, the specific restrictions imposed on the cell parameters by each crystal family become particularly simple. They are listed in columns 6 and 7 of Table 2.1.1.1. If within these restrictions the smallest cell is chosen, a *conventional* (crystallographic) *basis* results. Together with the selection of an appropriate *conventional* (crystallographic) *origin* (*cf.* Sections 2.1.3.2 and 2.1.3.7), such a basis defines a *conventional* (crystallographic) *coordinate system* and a *conventional cell.* The conventional cell of a point lattice or a space group, obtained in this way, turns out to be either *primitive* or to exhibit one of the *centring types* listed in Table 2.1.1.2. The centring type of a conventional cell is transferred to the lattice which is described by this cell; hence, we speak of primitive, face-centred, body-centred *etc.* lattices. Similarly, the cell parameters are often called lattice parameters; *cf.* Chapters 1.3 and 3.1 for further details.

In the triclinic, monoclinic and orthorhombic crystal systems, additional conventions (for instance cell reduction or metrical

Table 2.1.1.2
Symbols for the conventional centring types of one-, two- and three-dimensional cells

Symbol	Centring type of cell	Number of lattice points per cell	Coordinates of lattice points within cell
One dimension			
p	Primitive	1	0
Two dimensions			
p	Primitive	1	0, 0
c	Centred	2	0, 0; $\frac{1}{2}, \frac{1}{2}$
h†	Hexagonally centred	3	0, 0; $\frac{2}{3}, \frac{1}{3}$, $\frac{1}{3}, \frac{2}{3}$
Three dimensions			
P	Primitive	1	0, 0, 0
C	C-face centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}$, 0
A	A-face centred	2	0, 0, 0; 0, $\frac{1}{2}, \frac{1}{2}$
B	B-face centred	2	0, 0, 0; $\frac{1}{2}$, 0, $\frac{1}{2}$
I	Body centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
F	All-face centred	4	0, 0, 0; $\frac{1}{2}, \frac{1}{2}$, 0; 0, $\frac{1}{2}, \frac{1}{2}$, $\frac{1}{2}$, 0, $\frac{1}{2}$
R‡	Rhombohedrally centred (description with 'hexagonal axes')	3	0, 0, 0; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ ('obverse setting') 0, 0, 0; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$ ('reverse setting')
	Primitive (description with 'rhombohedral axes')	1	0, 0, 0
H§	Hexagonally centred	3	0, 0, 0; $\frac{2}{3}, \frac{1}{3}$, 0; $\frac{1}{3}, \frac{2}{3}$, 0

† The two-dimensional triple hexagonal cell h is an alternative description of the hexagonal plane net, as illustrated in Fig. 1.5.1.8. It is not used for systematic plane-group description in this volume; it is introduced, however, in the sub- and supergroup entries of the plane-group tables of *International Tables for Crystallography*, Vol. A1 (2010), abbreviated as *IT* A1. Plane-group symbols for the h cell are listed in Section 1.5.4. Transformation matrices are contained in Table 1.5.1.1.
‡ In the space-group tables (Chapter 2.3), as well as in *IT* (1935) and *IT* (1952), the seven rhombohedral R space groups are presented with two descriptions, one based on *hexagonal axes* (triple cell), one on *rhombohedral axes* (primitive cell). In the present volume, as well as in *IT* (1952) and *IT* A (2002), the *obverse* setting of the triple hexagonal cell R is used. Note that in *IT* (1935) the *reverse* setting was employed. The two settings are related by a rotation of the hexagonal cell with respect to the rhombohedral lattice around a threefold axis, involving a rotation angle of 60, 180 or 300° (*cf.* Fig. 1.5.1.6). Further details may be found in Section 1.5.4 and Chapter 3.1. Transformation matrices are contained in Table 1.5.1.1.
§ The triple hexagonal cell H is an alternative description of the hexagonal Bravais lattice, as illustrated in Fig. 1.5.1.8. It was used for systematic space-group description in *IT* (1935), but replaced by P in *IT* (1952). It is used in the tables of maximal subgroups and minimal supergroups of the space groups in *IT* A1 (2010). Space-group symbols for the H cell are listed in Section 1.5.4. Transformation matrices are contained in Table 1.5.1.1.

conventions based on the lengths of the cell edges) are needed to determine the choice and the labelling of the axes. Reduced bases are treated in Chapter 3.1, orthorhombic settings in Section 2.1.3.6, and monoclinic settings and cell choices in Section 2.1.3.15 (*cf.* Section 1.5.4 for a detailed treatment of alternative settings of space groups).

In this volume, all space groups within a crystal family are referred to the same kind of conventional coordinate system, with the exception of the hexagonal crystal family in three dimensions. Here, two kinds of coordinate systems are used, the hexagonal and the rhombohedral systems. In accordance with common crystallographic practice, all space groups based on the hexagonal Bravais lattice hP (18 trigonal and 27 hexagonal space groups) are described only with a hexagonal coordinate system (primitive cell), whereas the seven space groups based on the rhombohedral Bravais lattice hR (the so-called 'rhombohedral space groups', *cf.* Section 1.4.1) are treated in two versions, one referred to 'hexagonal axes' (triple obverse cell) and one to 'rhombohedral axes' (primitive cell); *cf.* Table 2.1.1.2. In practice, hexagonal axes are preferred because they are easier to visualize.

Table 2.1.1.2 contains only those conventional centring symbols which occur in the Hermann–Mauguin space-group symbols. There exist, of course, further kinds of centred cells which are unconventional, see for example the synoptic tables of plane (Table 1.5.4.3) and space (Table 1.5.4.4) groups discussed in Chapter 1.5. The centring type of a cell may change with a change of the basis vectors; in particular, a primitive cell may become a centred cell and *vice versa*. Examples of relevant transformation matrices are contained in Table 1.5.1.1.

2.1.2. Symbols of symmetry elements

By Th. Hahn and M. I. Aroyo

As already introduced in Section 1.2.3, a 'symmetry element' (of a given structure or object) is defined as a concept with two components; it is the combination of a 'geometric element' (that allows the fixed points of a reduced symmetry operation to be located and oriented in space) with the set of symmetry operations having this geometric element in common ('element set'). The element set of a symmetry element is represented by the so-called 'defining operation', which is the simplest symmetry operation from the element set that suffices to identify the geometric element. The alphanumeric and graphical symbols of symmetry elements and the related symmetry operations used throughout the tables of plane (Chapter 2.2) and space groups (Chapter 2.3) are listed in Tables 2.1.2.1 to 2.1.2.7. For detailed discussion of the definition and symbols of symmetry elements, *cf.* Section 1.2.3, de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000).

The alphanumeric symbols shown in Table 2.1.2.1 correspond to those symmetry elements and symmetry operations which occur in the conventional Hermann–Mauguin symbols of point groups and space groups. Further so-called 'additional symmetry elements' are described in Sections 1.4.2.3 and 1.5.4.1, and Tables 1.5.4.3 and 1.5.4.4 show additional symmetry operations that appear in the so-called 'extended Hermann–Mauguin symbols' (*cf.* Section 1.5.4). The symbols of symmetry elements (symmetry operations), except for glide planes (glide reflections), are independent of the choice and the labelling of the basis vectors and of the origin. The symbols of glide planes (glide reflections),

Table 2.1.2.1
Symbols for symmetry elements and for the corresponding symmetry operations in one, two and three dimensions

Symbol	Symmetry element and its orientation	Defining symmetry operation with glide or screw vector
m	Reflection plane, mirror plane	Reflection through the plane
	Reflection line, mirror line (two dimensions)	Reflection through the line
	Reflection point, mirror point (one dimension)	Reflection through the point
a, b or c	'Axial' glide plane	Glide reflection through the plane, with glide vector
a	$\perp$ [010] or $\perp$ [001]	$\frac{1}{2}\mathbf{a}$
b	$\perp$ [001] or $\perp$ [100]	$\frac{1}{2}\mathbf{b}$
c †	$\perp$ [100] or $\perp$ [010]	$\frac{1}{2}\mathbf{c}$
	$\perp$ [1$\bar{1}$0] or $\perp$ [110]	$\frac{1}{2}\mathbf{c}$
	$\perp$ [100] or $\perp$ [010] or $\perp$ [$\bar{1}\bar{1}$0]	$\frac{1}{2}\mathbf{c}$ } hexagonal coordinate system
	$\perp$ [1$\bar{1}$0] or $\perp$ [120] or $\perp$ [2$\bar{1}$0]	$\frac{1}{2}\mathbf{c}$ } hexagonal coordinate system
e ‡	'Double' glide plane (in centred cells only)	*Two* glide reflections through *one* plane, with perpendicular glide vectors
	$\perp$ [001]	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{b}$
	$\perp$ [100]	$\frac{1}{2}\mathbf{b}$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp$ [010]	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp$ [1$\bar{1}$0]; $\perp$ [110]	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$; $\frac{1}{2}(\mathbf{a}-\mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp$ [01$\bar{1}$]; $\perp$ [011]	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$; $\frac{1}{2}(\mathbf{b}-\mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$
	$\perp$ [$\bar{1}$01]; $\perp$ [101]	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$; $\frac{1}{2}(\mathbf{a}-\mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$
n	'Diagonal' glide plane	Glide reflection through the plane, with glide vector
	$\perp$ [001]; $\perp$ [100]; $\perp$ [010]	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$; $\frac{1}{2}(\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}+\mathbf{c})$
	$\perp$ [1$\bar{1}$0] or $\perp$ [01$\bar{1}$] or $\perp$ [$\bar{1}$01]	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
	$\perp$ [110]; $\perp$ [011]; $\perp$ [101]	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$
d §	'Diamond' glide plane	Glide reflection through the plane, with glide vector
	$\perp$ [001]; $\perp$ [100]; $\perp$ [010]	$\frac{1}{4}(\mathbf{a}\pm\mathbf{b})$; $\frac{1}{4}(\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}+\mathbf{c})$
	$\perp$ [1$\bar{1}$0]; $\perp$ [01$\bar{1}$]; $\perp$ [$\bar{1}$01]	$\frac{1}{4}(\mathbf{a}+\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}+\mathbf{b}+\mathbf{c})$; $\frac{1}{4}(\mathbf{a}\pm\mathbf{b}+\mathbf{c})$
	$\perp$ [110]; $\perp$ [011]; $\perp$ [101]	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}-\mathbf{b}+\mathbf{c})$; $\frac{1}{4}(\mathbf{a}\pm\mathbf{b}-\mathbf{c})$
g	Glide line (two dimensions)	Glide reflection through the line, with glide vector
	$\perp$ [01]; $\perp$ [10]	$\frac{1}{2}\mathbf{a}$; $\frac{1}{2}\mathbf{b}$
1	None	Identity
2, 3, 4, 6	n-fold rotation axis, n	Counter-clockwise rotation of 360/n degrees around the axis
	n-fold rotation point, n (two dimensions)	Counter-clockwise rotation of 360/n degrees around the point
$\bar{1}$	Centre of symmetry, inversion centre	Inversion through the point
$\bar{2}=m$, ¶ $\bar{3}$, $\bar{4}$, $\bar{6}$	Rotoinversion axis, $\bar{n}$, and inversion point on the axis ††	Counter-clockwise rotation of 360/n degrees around the axis, followed by inversion through the point on the axis ††
2_1	n-fold screw axis, n_p	Right-handed screw rotation of 360/n degrees around the axis, with screw vector (pitch) (p/n) **t**; here **t** is the shortest lattice translation vector parallel to the axis in the direction of the screw
3_1, 3_2		
4_1, 4_2, 4_3		
6_1, 6_2, 6_3, 6_4, 6_5		

† In the rhombohedral space-group symbols *R*3*c* (161) and *R*$\bar{3}$*c* (167), the symbol *c* refers to the description with 'hexagonal axes'; *i.e.* the glide vector is $\frac{1}{2}\mathbf{c}$, along [001]. In the description with 'rhombohedral axes', this glide vector is $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, along [111], *i.e.* the symbol of the glide plane would be *n: cf.* Table 1.5.4.4.
‡ Glide planes '*e*' occur in orthorhombic *A*-, *C*- and *F*-centred space groups, tetragonal *I*-centred and cubic *F*- and *I*-centred space groups. The geometric element of an *e*-glide plane is a plane shared by glide reflections with perpendicular glide vectors, with at least one glide vector along a crystal axis [*cf.* Section 1.2.3 and de Wolff *et al.* (1992)].
§ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{4}(\mathbf{a}-\mathbf{b})$. The second power of a glide reflection *d* is a centring vector.
¶ Only the symbol *m* is used in the Hermann–Mauguin symbols, for both point groups and space groups.
†† The inversion point is a centre of symmetry if *n* is odd.

however, may change with a change of the basis vectors. For this reason, the possible orientations of glide planes and the glide vectors of the corresponding operations are listed explicitly in columns 2 and 3 of Table 2.1.2.1.

In 1992, following a proposal of the Commission on Crystallographic Nomenclature (de Wolff *et al.*, 1992), the International Union of Crystallography introduced the symbol '*e*' and graphical symbols for the designation of the so-called 'double' glide planes. The double- or *e*-glide plane occurs only in centred cells and its geometric element is a plane shared by glide reflections with perpendicular glide vectors related by a centring translation (for details on *e*-glide planes, *cf.* Section 1.2.3). The introduction of the symbol *e* for the designation of double-glide planes (*cf.* de Wolff *et al.*, 1992) results in the modification of the Hermann–Mauguin symbols of five orthorhombic groups:

Space group No.	39	41	64	67	68
New symbol:	*Aem*2	*Aea*2	*Cmce*	*Cmme*	*Ccce*
Former symbol:	*Abm*2	*Aba*2	*Cmca*	*Cmma*	*Ccca*

Since the introduction of its use in *IT* A (2002) the new symbol is the standard one; it is indicated in the headline of these space groups, while the former symbol is given underneath.

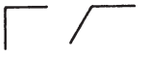
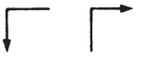
The graphical symbols of symmetry planes are shown in Tables 2.1.2.2 to 2.1.2.4. Like the alphanumeric symbols, the graphical symbols and their explanations (columns 2 and 3) are indepen-

Table 2.1.2.2
Graphical symbols of symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)

Description	Graphical symbol	Glide vector(s) of the defining operation(s) of the glide plane (in units of the shortest lattice translation vectors parallel and normal to the projection plane)	Symmetry element represented by the graphical symbol
Reflection plane, mirror plane Reflection line, mirror line (two dimensions)		None	*m*
'Axial' glide plane Glide line (two dimensions)		$\frac{1}{2}$ parallel to line in projection plane $\frac{1}{2}$ parallel to line in figure plane	*a*, *b* or *c* *g*
'Axial' glide plane		$\frac{1}{2}$ normal to projection plane	*a*, *b* or *c*
'Double' glide plane†		*Two* glide vectors: $\frac{1}{2}$ parallel to line in, and $\frac{1}{2}$ normal to projection plane	*e*
'Diagonal' glide plane		*One* glide vector with *two* components: $\frac{1}{2}$ parallel to line in, and $\frac{1}{2}$ normal to projection plane	*n*
'Diamond' glide plane‡ (pair of planes)		$\frac{1}{4}$ parallel to line in projection plane, combined with $\frac{1}{4}$ normal to projection plane (arrow indicates direction parallel to the projection plane for which the normal component is positive)	*d*

† The graphical symbols of the '*e*'-glide planes are applied to the diagrams of seven orthorhombic *A*-, *C*- and *F*-centred space groups, five tetragonal *I*-centred space groups, and five cubic *F*- and *I*-centred space groups.
‡ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{4}(\mathbf{a}-\mathbf{b})$. The second power of a glide reflection *d* is a centring vector.

Table 2.1.2.3
Graphical symbols of symmetry planes parallel to the plane of projection

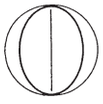
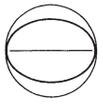
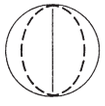
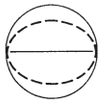
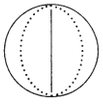
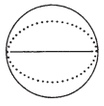
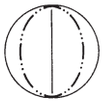
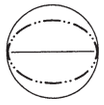
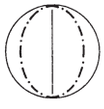
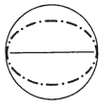
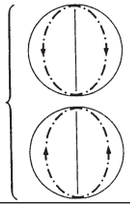
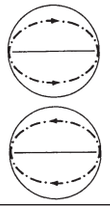
Description	Graphical symbol†	Glide vector(s) of the defining operation(s) of the glide plane (in units of the shortest lattice translation vectors parallel to the projection plane)	Symmetry element represented by the graphical symbol
Reflection plane, mirror plane		None	*m*
'Axial' glide plane		$\frac{1}{2}$ in the direction of the arrow	*a*, *b* or *c*
'Double' glide plane‡		*Two* glide vectors: $\frac{1}{2}$ in either of the directions of the two arrows	*e*
'Diagonal' glide plane		*One* glide vector with *two* components $\frac{1}{2}$ in the direction of the arrow	*n*
'Diamond' glide plane§ (pair of planes)		$\frac{1}{2}$ in the direction of the arrow; the glide vector is always half of a centring vector, *i.e.* one quarter of a diagonal of the conventional face-centred cell	*d*

† The symbols are given at the upper left corner of the space-group diagrams. A fraction *h* attached to a symbol indicates two symmetry planes with 'heights' *h* and $h+\frac{1}{2}$ above the plane of projection; *e.g.* $\frac{1}{8}$ stands for $h=\frac{1}{8}$ and $\frac{5}{8}$. No fraction means $h=0$ and $\frac{1}{2}$ (*cf.* Section 2.1.3.6).
‡ The graphical symbols of the '*e*'-glide planes are applied to the diagrams of seven orthorhombic *A*-, *C*- and *F*-centred space groups, five tetragonal *I*-centred space groups, and five cubic *F*- and *I*-centred space groups.
§ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{4}(\mathbf{a}-\mathbf{b})$. The second power of a glide reflection *d* is a centring vector.

dent of the projection direction and the labelling of the basis vectors. They are, therefore, applicable to any projection diagram of a space group. The alphanumeric symbols of glide planes (column 4), however, may change with a change of the basis vectors. For example, the dash-dotted *n* glide in the hexagonal description becomes an *a*, *b* or *c* glide in the rhombohedral description. In monoclinic space groups, the 'parallel' vector of a glide plane may be along a lattice translation vector that is inclined to the projection plane.

The '*e*'-glide graphical symbols are applied to the diagrams of seven orthorhombic *A*-, *C*- and *F*- centred space groups, five tetragonal *I*-centred space groups, and five cubic *F*- and *I*-centred space groups. The 'double-dotted-dash' symbol for *e* glides 'normal' and 'inclined' to the plane of projection was introduced

Table 2.1.2.4
Graphical symbols of symmetry planes inclined to the plane of projection (in cubic space groups of classes $\bar{4}3m$ and $m\bar{3}m$ only)

Description	Graphical symbol† for planes normal to		Glide vector(s) (in units of the shortest lattice translation vectors) of the defining operation(s) of the glide plane normal to		Symmetry element represented by the graphical symbol
	[011] and [01$\bar{1}$]	[101] and [10$\bar{1}$]	[011] and [01$\bar{1}$]	[101] and [10$\bar{1}$]	
Reflection plane, mirror plane			None	None	*m*
'Axial' glide plane			$\frac{1}{2}$ along [100]	$\frac{1}{2}$ along [010]	*a* or *b*
'Axial' glide plane			$\frac{1}{2}$ along [01$\bar{1}$] or along [011]	$\frac{1}{2}$ along [10$\bar{1}$] or along [101]	
'Double' glide plane [in space groups $I\bar{4}3m$ (217) and $Im\bar{3}m$ (229) only]			*Two* glide vectors: $\frac{1}{2}$ along [100] *and* $\frac{1}{2}$ along [01$\bar{1}$] or $\frac{1}{2}$ along [011]	*Two* glide vectors: $\frac{1}{2}$ along [010] *and* $\frac{1}{2}$ along [10$\bar{1}$] or $\frac{1}{2}$ along [101]	*e*
'Diagonal' glide plane			*One* glide vector: $\frac{1}{2}$ along [11$\bar{1}$] or along [111]‡	*One* glide vector: $\frac{1}{2}$ along [11$\bar{1}$] or along [111]‡	*n*
'Diamond' glide plane§ (pair of planes)			$\frac{1}{2}$ along [1$\bar{1}$1] or along [111]¶ $\frac{1}{2}$ along [$\bar{1}\bar{1}$1] or along [$\bar{1}$11]¶	$\frac{1}{2}$ along [$\bar{1}$11] or along [111] $\frac{1}{2}$ along [$\bar{1}\bar{1}$1] or along [1$\bar{1}$1] ¶	*d*

† The symbols represent orthographic projections. In the cubic space-group diagrams, complete orthographic projections of the symmetry elements around high-symmetry points, such as 0, 0, 0; $\frac{1}{2}$, 0, 0; $\frac{1}{4}$, $\frac{1}{4}$, 0, are given as 'inserts'.
‡ In the space groups $F\bar{4}3m$ (216), $Fm\bar{3}m$ (225) and $Fd\bar{3}m$ (227), the shortest lattice translation vectors in the glide directions are $\mathbf{t}(1,\frac{1}{2},\frac{\bar{1}}{2})$ or $\mathbf{t}(1,\frac{1}{2},\frac{1}{2})$ and $\mathbf{t}(\frac{1}{2},1,\frac{\bar{1}}{2})$ or $\mathbf{t}(\frac{1}{2},1,\frac{1}{2})$, respectively.
§ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{4}(\mathbf{a}-\mathbf{b})$. The second power of a glide reflection *d* is a centring vector.
¶ The glide vector is half of a centring vector, *i.e.* one quarter of the diagonal of the conventional body-centred cell in space groups $I\bar{4}3d$ (220) and $Ia\bar{3}d$ (230).

in 1992 (de Wolff *et al.*, 1992), while the 'double-arrowed' graphical symbol for *e*-glide planes oriented 'parallel' to the projection plane had already been used in *IT* (1935) and *IT* (1952).

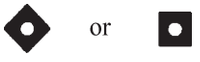
The graphical symbols of symmetry axes and their descriptions are shown in Tables 2.1.2.5–2.1.2.7. The screw vectors of the defining operations of screw axes are given in units of the shortest lattice translation vectors parallel to the axes. The symbols in the last column of the tables indicate the symmetry elements that are represented by the graphical symbols in the symmetry-element diagrams of the space groups. Two main cases may be distinguished:

(i) graphical symbols of symmetry elements that in the space-group diagrams represent just one symmetry element. Thus, the graphical symbol of a fourfold rotation axis or an inversion centre represent the symmetry element 4 or $\bar{1}$. Similarly, the graphical symbols of symmetry planes (Tables 2.1.2.2–2.1.2.4) represent just one symmetry element (namely, mirror or glide plane) in the space-group diagrams;

(ii) graphical symbols of symmetry elements that in the space-group diagrams represent more than one symmetry element. For example, the graphical symbol described in Table 2.1.2.5 as 'Inversion axis: 3 bar' ($\bar{3}$),

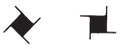
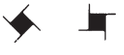
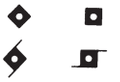
represents in the diagrams the three different symmetry elements $\bar{3}$, 3, $\bar{1}$.

The last six entries of Table 2.1.2.5 are combinations of symbols of symmetry axes with that of a centre of inversion. When displayed on the space-group diagrams, the combined graphical symbols represent more than one symmetry element. For example, the symbol for a fourfold rotation axis with a centre of inversion (4/*m*),



represents the symmetry elements $\bar{4}$, 4 and $\bar{1}$.

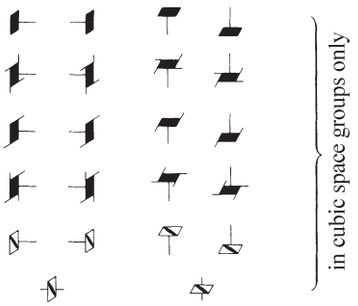
Table 2.1.2.5
Graphical symbols of symmetry axes normal to the plane of projection and symmetry points in the plane of the figure

Description	Alphanumeric symbol	Graphical symbol†	Screw vector of the defining operation of the screw axis (in units of the shortest lattice translation vector parallel to the axis)	Symmetry elements represented by the graphical symbol
Twofold rotation axis Twofold rotation point (two dimensions)	2		None	2
Twofold screw axis: '2 sub 1'	2_1		$\frac{1}{2}$	2_1
Threefold rotation axis Threefold rotation point (two dimensions)	3		None	3
Threefold screw axis: '3 sub 1'	3_1		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'	3_2		$\frac{2}{3}$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)	4		None	4
Fourfold screw axis: '4 sub 1'	4_1		$\frac{1}{4}$	4_1
Fourfold screw axis: '4 sub 2'	4_2		$\frac{1}{2}$	4_2
Fourfold screw axis: '4 sub 3'	4_3		$\frac{3}{4}$	4_3
Sixfold rotation axis Sixfold rotation point (two dimensions)	6		None	6
Sixfold screw axis: '6 sub 1'	6_1		$\frac{1}{6}$	6_1
Sixfold screw axis: '6 sub 2'	6_2		$\frac{1}{3}$	6_2
Sixfold screw axis: '6 sub 3'	6_3		$\frac{1}{2}$	6_3
Sixfold screw axis: '6 sub 4'	6_4		$\frac{2}{3}$	6_4
Sixfold screw axis: '6 sub 5'	6_5		$\frac{5}{6}$	6_5
Centre of symmetry, inversion centre: '1 bar' Reflection point, mirror point (one dimension)	$\bar{1}$		None	$\bar{1}$
Inversion axis: '3 bar'	$\bar{3}$		None	$\bar{3}$, $\bar{1}$, 3
Inversion axis: '4 bar'	$\bar{4}$		None	$\bar{4}$, 2
Inversion axis: '6 bar'	$\bar{6}$		None	$\bar{6}$, 3
Twofold rotation axis with centre of symmetry	$2/m$		None	2, $\bar{1}$
Twofold screw axis with centre of symmetry	$2_1/m$		$\frac{1}{2}$	2_1, $\bar{1}$
Fourfold rotation axis with centre of symmetry	$4/m$		None	4, $\bar{4}$, $\bar{1}$
'4 sub 2' screw axis with centre of symmetry	$4_2/m$		$\frac{1}{2}$	4_2, $\bar{4}$, $\bar{1}$
Sixfold rotation axis with centre of symmetry	$6/m$		None	6, $\bar{6}$, $\bar{3}$, $\bar{1}$
'6 sub 3' screw axis with centre of symmetry	$6_3/m$		$\frac{1}{2}$	6_3, $\bar{6}$, $\bar{3}$, $\bar{1}$

† Notes on the 'heights' h of symmetry points $\bar{1}$, $\bar{3}$, $\bar{4}$ and $\bar{6}$:
(1) Centres of symmetry $\bar{1}$ and $\bar{3}$, as well as inversion points $\bar{4}$ and $\bar{6}$ on $\bar{4}$ and $\bar{6}$ axes parallel to [001], occur in pairs at 'heights' h and $h+\frac{1}{2}$. In the space-group diagrams, only one fraction h is given, *e.g.* $\frac{1}{4}$ stands for $h=\frac{1}{4}$ and $\frac{3}{4}$. No fraction means $h=0$ and $\frac{1}{2}$. In *cubic* space groups, however, because of their complexity, *both* fractions are given for vertical $\bar{4}$ axes, including $h=0$ and $\frac{1}{2}$.
(2) Symmetries $4/m$ and $6/m$ contain vertical $\bar{4}$ and $\bar{6}$ axes; their $\bar{4}$ and $\bar{6}$ inversion points coincide with the centres of symmetry. This is not indicated in the space-group diagrams.
(3) Symmetries $4_2/m$ and $6_3/m$ also contain vertical $\bar{4}$ and $\bar{6}$ axes, but their $\bar{4}$ and $\bar{6}$ inversion points alternate with the centres of symmetry; *i.e.* $\bar{1}$ points at h and $h+\frac{1}{2}$ interleave with $\bar{4}$ or $\bar{6}$ points at $h+\frac{1}{4}$ and $h+\frac{3}{4}$. In the tetragonal and hexagonal space-group diagrams, only *one* fraction for $\bar{1}$ and one for $\bar{4}$ or $\bar{6}$ is given. In the cubic diagrams, *all four* fractions are listed for $4_2/m$; *e.g.* $Pm\bar{3}n$ (223): $\bar{1}$: 0, $\frac{1}{2}$; $\bar{4}$: $\frac{1}{4}$, $\frac{3}{4}$.

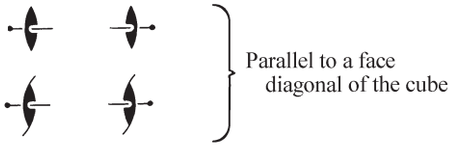
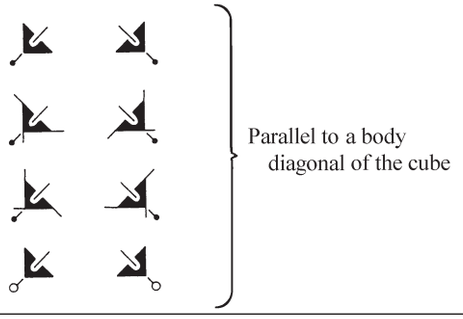
The meaning of a graphical symbol on the space-group diagrams is often confused with the set of symmetry elements that constitute the site-symmetry group associated with the symmetry element displayed. As an example, consider the rotoinversion axis $\bar{6}$ (described as 'Inversion axis: 6 bar' in Table 2.1.2.5). The site-symmetry group $\bar{6}$ can be decomposed into three symmetry elements: $\bar{6}$, 3 and m (*cf.* de Wolff *et al.*, 1989). However, the graphical symbol of $\bar{6}$ in the diagrams represents the two symmetry elements $\bar{6}$ and 3, as the symmetry element 'm' (that 'belongs' to $\bar{6}$) is represented by a separate graphical symbol.

Table 2.1.2.6
Graphical symbols of symmetry axes parallel to the plane of projection

Description	Graphical symbol†	Screw vector of the defining operation of the screw axis (in units of the shortest lattice translation vector parallel to the axis)	Symmetry elements represented by the graphical symbol
Twofold rotation axis		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Fourfold rotation axis		None	4
Fourfold screw axis: '4 sub 1'		$\frac{1}{4}$	4_1
Fourfold screw axis: '4 sub 2'		$\frac{1}{2}$	4_2
Fourfold screw axis: '4 sub 3'		$\frac{3}{4}$	4_3
Inversion axis: '4 bar'		None	$\bar{4}$, 2
Inversion point on '4 bar' axis		None	None

† The symbols for horizontal symmetry axes are given outside the unit cell of the space-group diagrams. *Twofold* axes always occur in pairs, at 'heights' h and $h + \frac{1}{2}$ above the plane of projection; here, a fraction h attached to such a symbol indicates two axes with heights h and $h + \frac{1}{2}$. No fraction stands for $h = 0$ and $\frac{1}{2}$. The rule of pairwise occurrence, however, is not valid for the horizontal *fourfold* axes in cubic space groups; here, *all* heights are given, including $h = 0$ and $\frac{1}{2}$. This applies also to the horizontal $\bar{4}$ axes and the $\bar{4}$ inversion points located on these axes.

Table 2.1.2.7
Graphical symbols of symmetry axes inclined to the plane of projection (in cubic space groups only)

Description	Graphical symbol†	Screw vector of the defining operation of the screw axis (in units of the shortest lattice translation vector parallel to the axis)	Symmetry elements represented by the graphical symbol
Twofold rotation axis		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Threefold rotation axis		None	3
Threefold screw axis: '3 sub 1'		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'		$\frac{2}{3}$	3_2
Inversion axis: '3 bar'		None	$\bar{3}$, 3, $\bar{1}$

† The dots mark the intersection points of axes with the plane at $h = 0$. In some cases, the intersection points are obscured by symbols of symmetry elements with height $h \geq 0$; examples: $Fd\bar{3}$ (203), origin choice 2; $Pn\bar{3}n$ (222), origin choice 2; $Pm\bar{3}n$ (223); $Im\bar{3}m$ (229); $Ia\bar{3}d$ (230).

2.1.3. Contents and arrangement of the tables

By Th. Hahn and A. Looijenga-Vos

2.1.3.1. General layout

The presentation of the plane-group and space-group data in Chapters 2.2 and 2.3 follows the style of the previous editions of *International Tables*. The data for most of the space groups are displayed on one page or on two facing pages. A typical distribution of the data is shown below and is illustrated by the example of *Cccm* (66) provided inside the front and back covers.

Left-hand page:

(1) *Headline*
(2) Diagrams for the symmetry elements and the general position (for graphical symbols of symmetry elements see Section 2.1.2)
(3) *Origin*
(4) *Asymmetric unit*
(5) *Symmetry operations*

Right-hand page:

(6) *Headline* in abbreviated form
(7) *Generators selected*; this information is the basis for the order of the entries under *Symmetry operations* and *Positions*
(8) General and special *Positions*, with the following columns:
Multiplicity
Wyckoff letter
Site symmetry, given by the oriented site-symmetry symbol
Coordinates
Reflection conditions
Note: In a few space groups, two special positions with the same reflection conditions are printed on the same line
(9) *Symmetry of special projections* (not given for plane groups)

It is important to note that the symmetry data are displayed in the same sequence for all the space groups. The actual distribution of the data between pages can vary depending on the amount and nature of the data that are shown.

The symmetry data for the ten space groups of the crystal class $m\bar{3}m$ [$Pm\bar{3}m$ (221) to $Ia\bar{3}d$ (230)] are displayed on four pages. Additional general-position diagrams in tilted projection are shown on the fourth page, providing a three-dimensional-style view of these complicated general-position diagrams.

2.1.3.2. Space groups with more than one description

For several space groups, more than one description is available. Three cases occur:

(i) *Two choices of origin (cf. Section 2.1.3.7)*

For all centrosymmetric space groups, the tables contain a description with a centre of symmetry as origin. Some centrosymmetric space groups, however, contain points of high site symmetry that do not coincide with a centre of symmetry. For these 24 cases, a further description (including diagrams) with a high-symmetry point as origin is provided. Neither of the two origin choices is considered standard. Noncentrosymmetric space groups and all plane groups are described with only one choice of origin.

Examples

(1) *Pnnn* (48)
Origin choice 1 at a point with site symmetry 222
Origin choice 2 at a centre with site symmetry $\bar{1}$.
(2) $Fd\bar{3}m$ (227)
Origin choice 1 at a point with site symmetry $\bar{4}3m$
Origin choice 2 at a centre with site symmetry $\bar{3}m$.

(ii) *Monoclinic space groups*

Two complete descriptions are given for each of the 13 monoclinic space groups, one for the setting with 'unique axis *b*', followed by one for the setting with 'unique axis *c*'.

Additional descriptions in synoptic form are provided for the following eight monoclinic space groups with centred lattices or glide planes:

*C*2 (5), *Pc* (7), *Cm* (8), *Cc* (9), *C*2/*m* (12), *P*2/*c* (13), $P2_1/c$ (14), *C*2/*c* (15)

These synoptic descriptions consist of abbreviated treatments for three 'cell choices', here called 'cell choices 1, 2 and 3'. Cell choice 1 corresponds to the complete treatment, mentioned above; for comparative purposes, it is repeated among the synoptic descriptions which, for each setting, are printed on two facing pages. The cell choices and their relations are explained in Section 2.1.3.15.

(iii) *Rhombohedral space groups*

The seven rhombohedral space groups *R*3 (146), $R\bar{3}$ (148), *R*32 (155), *R*3*m* (160), *R*3*c* (161), $R\bar{3}m$ (166) and $R\bar{3}c$ (167) are described with two coordinate systems, first with *hexagonal axes* (triple hexagonal cell) and second with *rhombohedral axes* (primitive rhombohedral cell). The same space-group symbol is used for both descriptions. For convenience, the relations between the cell parameters a, c of the triple hexagonal cell and the cell parameters a' and α' of the primitive rhombohedral cell (*cf.* Table 2.1.1.1) are listed:

$$a = a'\sqrt{2}\sqrt{1-\cos\alpha'} = 2a'\sin\frac{\alpha'}{2}$$

$$c = a'\sqrt{3}\sqrt{1+2\cos\alpha'}$$

$$\frac{c}{a} = \sqrt{\frac{3}{2}}\sqrt{\frac{1+2\cos\alpha'}{1-\cos\alpha'}} = \sqrt{\frac{9}{4\sin^2(\alpha'/2)} - 3}$$

$$a' = \tfrac{1}{3}\sqrt{3a^2 + c^2}$$

$$\sin\frac{\alpha'}{2} = \frac{3}{2\sqrt{3 + (c^2/a^2)}} \text{ or } \cos\alpha' = \frac{(c^2/a^2) - \frac{3}{2}}{(c^2/a^2) + 3}.$$

The hexagonal triple cell is given in the *obverse* setting (centring points $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$). In *IT* (1935), the *reverse* setting (centring points $\frac{1}{3},\frac{2}{3},\frac{1}{3}$; $\frac{2}{3},\frac{1}{3},\frac{2}{3}$) was employed; *cf.* Table 2.1.1.2.

Coordinate transformations between different space-group descriptions are treated in detail in Section 1.5.3.

2.1.3.3. Headline

The description of each plane group or space group starts with a headline consisting of two (sometimes three) lines which contain the following information, when read from left to right.

First line

(1) The *short international* (Hermann–Mauguin) *symbol* for the plane or space group. These symbols will be further referred to as Hermann–Mauguin symbols. A detailed discussion of space-group symbols is given in Section 1.4.1 and Chapter 3.3; for convenience, a summary is given in Section 2.1.3.4.

Note on standard monoclinic space-group symbols: In order to facilitate recognition of a monoclinic space-group type, the familiar short symbol for the *b*-axis setting (*e.g.* $P2_1/c$ for No. 14 or $C2/c$ for No. 15) has been adopted as the *standard symbol* for a space-group type. It appears in the headline of *every description of this space group* and thus does not carry any information about the setting or the cell choice of this particular description. No other short symbols for monoclinic space groups are used in this volume (*cf.* Section 2.1.3.15).

(2) The *Schoenflies symbol* for the space group (*cf.* Section 1.4.1).

Note: No Schoenflies symbols exist for the plane groups.

(3) The *short international* (Hermann–Mauguin) *symbol* for the point group to which the plane or space group belongs (*cf.* Section 1.4.1 and Chapter 3.3).

(4) The name of the *crystal system* (*cf.* Table 2.1.1.1).

Second line

(5) The sequential *number of the plane or space group*, as introduced in *IT* (1952).

(6) The *full international* (Hermann–Mauguin) *symbol* for the plane or space group.

For monoclinic space groups, the headline of every description contains the full symbol appropriate to that description.

(7) The *Patterson symmetry* (see Section 2.1.3.5).

Third line

This line is used, where appropriate, to indicate origin choices, settings, cell choices and coordinate axes (see Section 2.1.3.2). For five orthorhombic space groups, an entry 'Former space-group symbol' is given; *cf.* Section 2.1.2.

Table 2.1.3.1
Lattice symmetry directions for two and three dimensions

Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.

	Symmetry direction (position in Hermann–Mauguin symbol)		
Lattice	Primary	Secondary	Tertiary
Two dimensions			
Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		{[10], [01]}	{[1$\bar{1}$], [11]}
Hexagonal		{[10], [01], [1$\bar{1}$]}	{[1$\bar{1}$], [12], [2$\bar{1}$]}
Three dimensions			
Triclinic	None		
Monoclinic†	[010] ('unique axis *b*') [001] ('unique axis *c*')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	{[100], [010]}	{[1$\bar{1}$0], [110]}
Hexagonal	[001]	{[100], [010], [1$\bar{1}$0]}	{[1$\bar{1}$0], [120], [2$\bar{1}$0]}
Rhombohedral (hexagonal axes)	[001]	{[100], [010], [1$\bar{1}$0]}	
Rhombohedral (rhombohedral axes)	[111]	{[1$\bar{1}$0], [01$\bar{1}$], [$\bar{1}$01]}	
Cubic	{[100], [010], [001]}	{[111], [1$\bar{1}$1], [$\bar{1}$11], [11$\bar{1}$]}	{[1$\bar{1}$0] [110], [01$\bar{1}$] [011], [$\bar{1}$01] [101]}

† For the full Hermann–Mauguin symbols see Sections 2.1.3.4 and 1.4.1.

2.1.3.4. International (Hermann–Mauguin) symbols for plane groups and space groups

(For more details, *cf.* Section 1.4.1 and Chapter 3.3.)

Current symbols. Both the short and the full Hermann–Mauguin symbols consist of two parts: (i) a letter indicating the centring type of the conventional cell, and (ii) a set of characters indicating symmetry elements of the space group (modified point-group symbol).

(i) The letters for the centring types of cells are listed in Table 2.1.1.2. Lower-case letters are used for two dimensions (nets), capital letters for three dimensions (lattices).

(ii) The one, two or three entries after the centring letter refer to the one, two or three kinds of *symmetry directions* of the lattice belonging to the space group. These symmetry directions were called *Blickrichtungen* by Heesch (1929). Symmetry directions occur either as singular directions (as in the monoclinic and orthorhombic crystal systems) or as sets of symmetry-equivalent symmetry directions (as in the higher-symmetry crystal systems). Only one representative of each set is required. The (sets of) symmetry directions and their sequence for the different lattices are summarized in Table 2.1.3.1. According to their position in this sequence, the symmetry directions are referred to as 'primary', 'secondary' and 'tertiary' directions.

This sequence of lattice symmetry directions is transferred to the sequence of positions in the corresponding Hermann–Mauguin space-group symbols. Each position contains one or two characters designating symmetry elements (axes and planes) of the space group (*cf.* Section 2.1.2) that occur for the corresponding lattice symmetry direction. Symmetry planes are represented by their normals; if a symmetry axis and a normal to a symmetry plane are parallel, the two characters (symmetry symbols) are separated by a slash, as in $P6_3/m$ or $P2/m$ ('two over *m*').

Short and *full* Hermann–Mauguin symbols differ only for the plane groups of class *m*, for the monoclinic space groups, and for the space groups of crystal classes *mmm*, $4/mmm$, $\bar{3}m$, $6/mmm$, $m\bar{3}$ and $m\bar{3}m$. In the full symbols, symmetry axes *and* symmetry

Table 2.1.3.2
Changes in Hermann–Mauguin symbols for two-dimensional groups

No.	*IT* (1952)	Present edition
6	*pmm*	*p*2*mm*
7	*pmg*	*p*2*mg*
8	*pgg*	*p*2*gg*
9	*cmm*	*c*2*mm*
11	*p*4*m*	*p*4*mm*
12	*p*4*g*	*p*4*gm*
17	*p*6*m*	*p*6*mm*

planes for each symmetry direction are listed; in the short symbols, symmetry axes are suppressed as much as possible. Thus, for space group No. 62, the full symbol is $P2_1/n\ 2_1/m\ 2_1/a$ and the short symbol is *Pnma*. For No. 194, the full symbol is $P6_3/m\ 2/m\ 2/c$ and the short symbol is $P6_3/mmc$. For No. 230, the full symbol is $I4_1/a\ \bar{3}\ 2/d$ and the short symbol is $Ia\bar{3}d$.

Many space groups contain more kinds of symmetry elements than are indicated in the full symbol ('additional symmetry operations and elements', *cf.* Sections 1.4.2.4 and 1.5.4.1). A listing of additional symmetry operations is given in Tables 1.5.4.3 and 1.5.4.4 under the heading *Extended full symbols*. Note that a centre of symmetry is never explicitly indicated (except for space group $P\bar{1}$); its presence or absence, however, can be readily inferred from the space-group symbol.

Changes in Hermann–Mauguin space-group symbols as compared with the 1952 and 1935 editions of International Tables. Extensive changes in the space-group symbols were applied in *IT* (1952) as compared with the original Hermann–Mauguin symbols of *IT* (1935), especially in the tetragonal, trigonal and hexagonal crystal systems. Moreover, new symbols for the *c*-axis setting of monoclinic space groups were introduced. All these changes are recorded on pp. 51 and 543–544 of *IT* (1952). In the present edition, the symbols of the 1952 edition are retained, except for the following four cases (*cf.* Section 3.3.4).

(i) *Two-dimensional groups*. Short Hermann–Mauguin symbols differing from the corresponding full symbols in *IT* (1952) are replaced by the full symbols for the plane groups listed in Table 2.1.3.2.

For the two-dimensional point group with two mutually perpendicular mirror lines, the symbol *mm* is changed to 2*mm*.

For plane group No. 2, the entries '1' at the end of the full symbol are omitted: No. 2: Change from *p*211 to *p*2.

With these changes, the symbols of the two-dimensional groups follow the rules that were introduced in *IT* (1952) for the space groups.

(ii) *Monoclinic space groups*. Additional *full* Hermann–Mauguin symbols are introduced for the eight monoclinic space groups with centred lattices or glide planes (Nos. 5, 7–9, 12–15) to indicate the various settings and cell choices. A complete list of symbols, including also the *a*-axis setting, is contained in Table 1.5.4.4; further details are given in Section 2.1.3.15.

For standard *short* monoclinic space-group symbols see Sections 2.1.3.3 and 2.1.3.15.

(iii) *Cubic space groups*. The short symbols for all space groups belonging to the two cubic crystal classes $m\bar{3}$ and $m\bar{3}m$ now contain the symbol $\bar{3}$ instead of 3. This applies to space groups Nos. 200–206 and 221–230, as well as to the two point groups $m\bar{3}$ and $m\bar{3}m$.

Examples

No. 205: Change from $Pa3$ to $Pa\bar{3}$

No. 230: Change from $Ia3d$ to $Ia\bar{3}d$.

With this change, the centrosymmetric nature of these groups is apparent also in the short symbols.

(iv) *Glide-plane symbol e*. For the introduction of the 'double glide plane' *e* into five space-group symbols, see Section 2.1.2.

2.1.3.5. Patterson symmetry

By H. D. Flack

The entry *Patterson symmetry* in the headline gives the symmetry of the 'vector set' generated by the operation of the space group on an arbitrary set of general positions. More prosaically, it may be described as the symmetry of the set of the interatomic vectors of a crystal structure with the selected space group. The Patterson symmetry is a crystallographic space group denoted by its Hermann–Mauguin symbol. It is in fact one of the 24 centrosymmetric symmorphic space groups (see Section 1.3.3.3) in three dimensions and one of 7 in two dimensions. For each of the 230 space groups, the Patterson symmetry has the same Bravais-lattice type as the space group itself and its point group is the lowest-index centrosymmetric supergroup of the point group of the space group. The 'point-group part' of the symbol of the Patterson symmetry represents the Laue class to which the plane group or space group belongs (*cf.* Table 2.1.2.1). By way of examples: space group No. 100, *P*4*bm*, has a Bravais lattice of type *tP* and point group 4*mm*. The centrosymmetric supergroup of 4*mm* (see Fig. 3.2.1.3) is 4/*mmm*, so the Patterson symmetry is *P*4/*mmm*; space group No. 66, *Cccm*, has a Bravais lattice of type *oC* and point group *mmm*. This point group is centrosymmetric, so the Patterson symmetry is *Cmmm*.

Note: For the four space groups *Amm*2 (38), *Aem*2 (39), *Ama*2 (40) and *Aea*2 (41), the standard symbol for their Patterson symmetry, *Cmmm*, is added (between parentheses) after the actual symbol *Ammm* in the space-group tables.

The Patterson symmetry is intimately related to the symmetry of the Patterson function (see Flack, 2015). The latter, $P_{|F|^2}(uvw)$, is the inverse Fourier transform of the squared structure-factor amplitudes. Patterson functions possess the crystallographic symmetry of the symmorphic space-group representative of the arithmetic crystal class (see Section 1.3.4.4.1) to which the space group belongs. Table 2.1.3.3 lists these crystallographic symmetries of the Patterson function and the Patterson symmetries for the space groups and plane groups. However, further symmetry is also present, as desribed below for the three common forms of the Patterson function:

(*a*) $P_{|F|^2}(uvw)$: The most general form of the Patterson function, the complex $P_{|F|^2}(uvw)$, is the complex Fourier transform of $|F(hkl)|^2$. The full symmetry of $P_{|F|^2}(uvw)$ can be described in terms of the 1651 two-colour (Shubnikov) space groups (Fischer & Knof, 1987; Wilson, 1993; Shubnikov & Belov, 1964; *cf.* also Chapter 3.6). The real and imaginary parts of $P_{|F|^2}(uvw)$ have the same symmetry as $P_A(uvw)$ and $P_D(uvw)$, respectively, described below. $P_{|F|^2}(uvw)$ is real for centrosymmetric space groups and noncentrosymmetric ones in the absence of any resonant-scattering contribution.

(*b*) $P_A(uvw)$: $A(hkl) = \frac{1}{2}[|F(hkl)|^2 + |F(\bar{h}\bar{k}\bar{l})|^2]$, the average of the squared structure-factor amplitudes of the pair of Friedel opposites *hkl* and $\bar{h}\bar{k}\bar{l}$. Real $P_A(uvw)$ is the real cosine Fourier

Table 2.1.3.3
Patterson symmetries and symmetries of Patterson functions for space groups and plane groups

The space-group types of each row form an arithmetic crystal class. (In three instances the row is typeset on two lines.) The arithmetic crystal class is identified by its representative symmorphic space group for which both the Hermann–Mauguin symbol and the space-group-type number are shown in bold. A set of space groups with sequential numbers is indicated by the symbols of the first and last space group of the sequence separated by a dash.

The column 'Patterson symmetry' indicates the symmetry of the set of interatomic vectors of crystal structures described in the space groups given in the column 'Space-group types'. The Patterson symmetry is also the symmetry of $P_A(uvw)$ and the real part of the complex $P_{|F|^2}(uvw)$. The Patterson symmetry is given in the headline of each space-group table in Chapter 2.3.

The crystallographic symmetry of both $P_D(uvw)$ and the imaginary part of the complex $P_{|F|^2}(uvw)$ is that of the symmorphic space group of crystal structures described in the space groups given in the column 'Space-group types'. To this crystallographic symmetry, the noncrystallographic operation of a centre of antisymmetry needs to be added to give $P_D(uvw) = -P_D(\bar{u}\bar{v}\bar{w})$. The full symmetry of $P_D(uvw)$ is not shown in this volume.

The setting and origin choice of the chosen space group should also be used for the space group of the Patterson symmetry and the symmorphic space group.

Similar remarks apply to the plane groups listed in part (*b*) of the table.

(*a*) Space groups.

Space-group types		Patterson symmetry
Hermann–Mauguin symbols	Nos.	
Crystal family triclinic (anorthic), Bravais-lattice type *aP*		
***P*1**	**1**	$P\bar{1}$
***P*$\bar{1}$**	**2**	$P\bar{1}$
Crystal family monoclinic, Bravais-lattice type *mP*		
***P*2**–$P2_1$	**3**–4	$P2/m$
Pm–Pc	**6**–7	$P2/m$
P*2/*m–$P2_1/m$, $P2/c$–$P2_1/c$	**10**–11, 13–14	$P2/m$
Crystal family monoclinic, Bravais-lattice type *mS*		
***C*2**	**5**	$C2/m$
Cm–Cc	**8**–9	$C2/m$
C*2/*m, $C2/c$	**12**, 15	$C2/m$
Crystal family orthorhombic, Bravais-lattice type *oP*		
***P*222**–$P2_12_12_1$	**16**–19	$Pmmm$
***Pmm*2**–$Pnn2$	**25**–34	$Pmmm$
Pmmm–$Pnma$	**47**–62	$Pmmm$
Crystal family orthorhombic, Bravais-lattice type *oS*		
$C222_1$, ***C*222**	20, **21**	$Cmmm$
***Cmm*2**–$Ccc2$	**35**–37	$Cmmm$
***Amm*2**–$Aea2$	**38**–41	$Ammm$
$Cmcm$–$Cmce$, ***Cmmm***, $Cccm$–$Ccce$	63–64, **65**, 66–68	$Cmmm$
Crystal family orthorhombic, Bravais-lattice type *oF*		
***F*222**	**22**	$Fmmm$
***Fmm*2**–$Fdd2$	**42**–43	$Fmmm$
Fmmm–$Fddd$	**69**–70	$Fmmm$
Crystal family orthorhombic, Bravais-lattice type *oI*		
***I*222**–$I2_12_12_1$	**23**–24	$Immm$
***Imm*2**–$Ima2$	**44**–46	$Immm$
Immm–$Imma$	**71**–74	$Immm$
Crystal family tetragonal, Bravais-lattice type *tP*		
***P*4**–$P4_3$	**75**–78	$P4/m$
***P*$\bar{4}$**	**81**	$P4/m$
P*4/*m–$P4_2/n$	**83**–86	$P4/m$
***P*422**–$P4_32_12$	**89**–96	$P4/mmm$
P*4*mm–$P4_2bc$	**99**–106	$P4/mmm$
P*$\bar{4}$2*m–$P\bar{4}2_1c$	**111**–114	$P4/mmm$
***P*$\bar{4}$*m*2**–$P\bar{4}n2$	**115**–118	$P4/mmm$
P*4/*mmm–$P4_2/ncm$	**123**–138	$P4/mmm$
Crystal family tetragonal, Bravais-lattice type *tI*		
***I*4**, $I4_1$	**79**–80	$I4/m$
***I*$\bar{4}$**	**82**	$I4/m$
I*4/*m–$I4_1/a$	**87**–88	$I4/m$
***I*422**–$I4_122$	**97**–98	$I4/mmm$
I*4*mm–$I4_1cd$	**107**–110	$I4/mmm$
***I*$\bar{4}$*m*2**–$I\bar{4}c2$	**119**–120	$I4/mmm$
I*$\bar{4}$2*m–$I\bar{4}2d$	**121**–122	$I4/mmm$
I*4/*mmm–$I4_1/acd$	**139**–142	$I4/mmm$
Crystal family hexagonal, Bravais-lattice type *hP*		
***P*3**–$P3_2$	**143**–145	$P\bar{3}$
***P*$\bar{3}$**	**147**	$P\bar{3}$
***P*312**, $P3_112$, $P3_212$	**149**, 151, 153	$P\bar{3}1m$
***P*321**, $P3_121$, $P3_221$	**150**, 152, 154	$P\bar{3}m1$
***P*3*m*1**, $P3c1$	**156**, 158	$P\bar{3}m1$
P*31*m, $P31c$	**157**, 159	$P\bar{3}1m$
P*$\bar{3}$1*m–$P\bar{3}1c$	**162**–163	$P\bar{3}1m$
***P*$\bar{3}$*m*1**–$P\bar{3}c1$	**164**–165	$P\bar{3}m1$
***P*6**–$P6_3$	**168**–173	$P6/m$
***P*$\bar{6}$**	**174**	$P6/m$
P*6/*m–$P6_3/m$	**175**–176	$P6/m$
***P*622**–$P6_322$	**177**–182	$P6/mmm$
P*6*mm–$P6_3mc$	**183**–186	$P6/mmm$
***P*$\bar{6}$*m*2**–$P\bar{6}c2$	**187**–188	$P6/mmm$
P*$\bar{6}$2*m–$P\bar{6}2c$	**189**–190	$P6/mmm$
P*6/*mmm–$P6_3/mmc$	**191**–194	$P6/mmm$
Crystal family hexagonal, Bravais-lattice type *hR*		
***R*3**	**146**	$R\bar{3}$
***R*$\bar{3}$**	**148**	$R\bar{3}$
***R*32**	**155**	$R\bar{3}m$
R*3*m–$R3c$	**160**–161	$R\bar{3}m$
R*$\bar{3}$*m–$R\bar{3}c$	**166**–167	$R\bar{3}m$
Crystal family cubic, Bravais-lattice type *cP*		
***P*23**, $P2_13$	**195**, 198	$Pm\bar{3}$
***Pm*$\bar{3}$**–$Pn\bar{3}$, $Pa\bar{3}$	**200**–201, 205	$Pm\bar{3}$
***P*432**–$P4_232$, $P4_332$–$P4_132$	**207**–208, 212–213	$Pm\bar{3}m$
P*$\bar{4}$3*m, $P\bar{4}3n$	**215**, 218	$Pm\bar{3}m$
Pm*$\bar{3}$*m–$Pn\bar{3}m$	**221**–224	$Pm\bar{3}m$

transform of $A(hkl)$. The symmetry of $P_A(uvw)$ is generated by the symmorphic space-group representative of the arithmetic crystal class to which the space group belongs, combined with a centre of symmetry (inversion centre), *i.e.* $P_A(uvw) = P_A(\bar{u}\bar{v}\bar{w})$. $P_A(uvw)$ thus possesses the Patterson symmetry of the space group whether the latter is centrosymmetric or not, and whether there is any resonant-scattering contribution or not (see Table 2.1.3.3).

Table 2.1.3.3 (continued)

Space-group types		
Hermann–Mauguin symbols	Nos.	Patterson symmetry
Crystal family cubic, Bravais-lattice type *cF*		
***F*23**	**196**	$Fm\bar{3}$
***Fm*$\bar{3}$**–$Fd\bar{3}$	**202**–203	$Fm\bar{3}$
***F*432**–$F4_132$	**209**–210	$Fm\bar{3}m$
F*$\bar{4}$3*m–$F\bar{4}3c$	**216**, 219	$Fm\bar{3}m$
Fm*$\bar{3}$*m–$Fd\bar{3}c$	**225**–228	$Fm\bar{3}m$
Crystal family cubic, Bravais-lattice type *cI*		
***I*23**, $I2_13$	**197**, 199	$Im\bar{3}$
***Im*$\bar{3}$**, $Ia\bar{3}$	**204**, 206	$Im\bar{3}$
***I*432**, $I4_132$	**211**, 214	$Im\bar{3}m$
I*$\bar{4}$3*m, $I\bar{4}3d$	**217**, 220	$Im\bar{3}m$
Im*$\bar{3}$*m–$Ia\bar{3}d$	**229**–230	$Im\bar{3}m$

(*b*) Plane groups.

Plane-group types		
Hermann–Mauguin symbols	Nos.	Patterson symmetry
Crystal family oblique (monoclinic), Bravais-lattice type *mp*		
***p*1**	**1**	*p*2
***p*2**	**2**	*p*2
Crystal family rectangular (orthorhombic), Bravais-lattice type *op*		
pm–*pg*	**3**–4	*p*2*mm*
p*2*mm–*p*2*gg*	**6**–8	*p*2*mm*
Crystal family rectangular (orthorhombic), Bravais-lattice type *oc*		
cm	**5**	*c*2*mm*
c*2*mm	**9**	*c*2*mm*
Crystal family square (tetragonal), Bravais-lattice type *tp*		
***p*4**	**10**	*p*4
p*4*mm–*p*4*gm*	**11**–12	*p*4*mm*
Crystal family hexagonal, Bravais-lattice type *hp*		
***p*3**	**13**	*p*6
***p*3*m*1**	**14**	*p*6*mm*
p*31*m	**15**	*p*6*mm*
***p*6**	**16**	*p*6
p*6*mm	**17**	*p*6*mm*

(*c*) $P_D(uvw)$: $D(hkl) = |F(hkl)|^2 - |F(\bar{h}\bar{k}\bar{l})|^2$, the difference of the squared structure-factor amplitudes of the pair of Friedel opposites hkl and $\bar{h}\bar{k}\bar{l}$. Real $P_D(uvw)$ is the real sine Fourier transform of $D(hkl)$. The crystallographic symmetry of $P_D(uvw)$ is that of the symmorphic space-group representative of the arithmetic crystal class to which the space group belongs (see Table 2.1.3.3). The full symmetry of $P_D(uvw)$ is given by the type-III black-and-white space group generated by the appropriate symmorphic space group and the *centre of antisymmetry*, $P_D(uvw) = -P_D(\bar{u}\bar{v}\bar{w})$ (Fischer & Knof, 1987). Thus $P_D(uvw)$ does not possess the Patterson symmetry.

2.1.3.6. Space-group diagrams

The space-group diagrams serve two purposes: (i) to show the relative locations and orientations of the symmetry elements and (ii) to illustrate the arrangement of a set of symmetry-equivalent points of the general position.

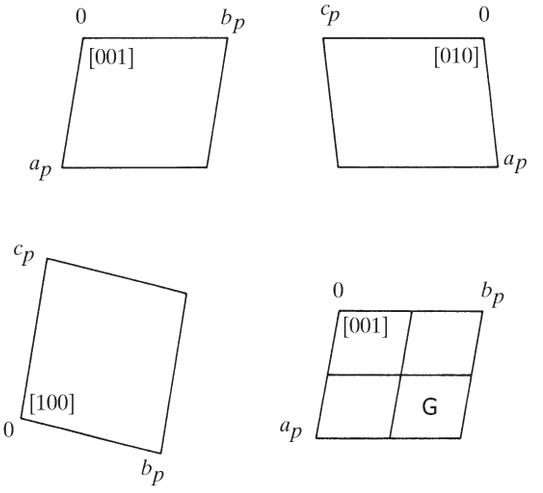


Figure 2.1.3.1
Triclinic space groups (G = general-position diagram).

With the exception of general-position diagrams in perspective projection for some space groups (*cf.* Section 2.1.3.6.8), all of the diagrams are orthogonal projections, *i.e.* the projection direction is perpendicular to the plane of the figure. Apart from the descriptions of the rhombohedral space groups with 'rhombohedral axes' (*cf.* Section 2.1.3.6.6), the projection direction is always a cell axis. If other axes are not parallel to the plane of the figure, they are indicated by the subscript p, as a_p, b_p or c_p in the case of one or two axes for monoclinic and triclinic space groups, respectively (*cf.* Figs. 2.1.3.1 to 2.1.3.3), or by the subscript rh for the three rhombohedral axes in Fig. 2.1.3.9.

The graphical symbols for symmetry elements, as used in the drawings, are displayed in Tables 2.1.2.2 to 2.1.2.7.

In the diagrams, 'heights' h above the projection plane are indicated for symmetry planes and symmetry axes *parallel* to the projection plane, as well as for centres of symmetry. The heights are given as fractions of the shortest lattice translation normal to the projection plane and, if different from 0, are printed next to the graphical symbols. Each symmetry element at height h is accompanied by another symmetry element of the same type at height $h + \frac{1}{2}$ (this does not apply to the horizontal fourfold axes in the diagrams for the cubic space groups). In the space-group diagrams, only the symmetry element at height h is indicated (*cf.* Section 2.1.2).

Schematic representations of the diagrams, displaying the origin, the labels of the axes, and the projection direction [*uvw*], are given in Figs. 2.1.3.1 to 2.1.3.10 (except Fig. 2.1.3.6). The general-position diagrams are indicated by the letter G.

2.1.3.6.1. Plane groups

Each description of a plane group contains two diagrams, one for the symmetry elements (left) and one for the general position (right). The two axes are labelled a and b, with a pointing downwards and b running from left to right.

2.1.3.6.2. Triclinic space groups

For each of the two triclinic space groups, three elevations (along a, b and c) are given, in addition to the general-position diagram G (projected along c) at the lower right of the set, as illustrated in Fig. 2.1.3.1.

The diagrams represent a reduced cell of type II for which the three interaxial angles are non-acute, *i.e.* $\alpha, \beta, \gamma \geq 90^\circ$. For a cell

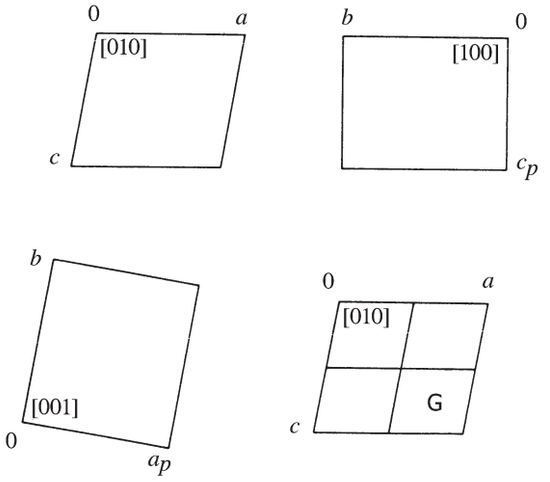


Figure 2.1.3.2
Monoclinic space groups, setting with unique axis *b* (G = general-position diagram).

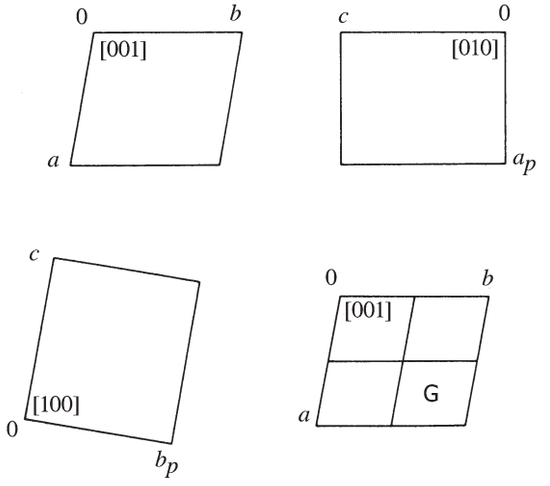


Figure 2.1.3.3
Monoclinic space groups, setting with unique axis *c* (G = general-position diagram).

of type I, all angles are acute, *i.e.* $\alpha, \beta, \gamma < 90°$. For a discussion of the two types of reduced cells, see Section 3.1.3.

2.1.3.6.3. Monoclinic space groups (cf. Sections 2.1.3.2 and 2.1.3.15)

The 'complete treatment' of each of the two settings contains four diagrams (Figs. 2.1.3.2 and 2.1.3.3). Three of them are projections of the symmetry elements, taken along the unique axis (upper left) and along the other two axes (lower left and upper right). For the general position, only the projection along the unique axis is given (lower right).

The 'synoptic descriptions' of the three cell choices (for each setting) are headed by a pair of diagrams, as illustrated in Fig. 2.1.3.4. The drawings on the left display the symmetry elements and the ones on the right the general position (labelled G). Each diagram is a projection of four neighbouring unit cells along the unique axis. It contains the outlines of the three cell choices drawn as heavy lines. For the labelling of the axes, see Fig. 2.1.3.4. The headline of the description of each cell choice contains a small-scale drawing, indicating the basis vectors and the cell that apply to that description.

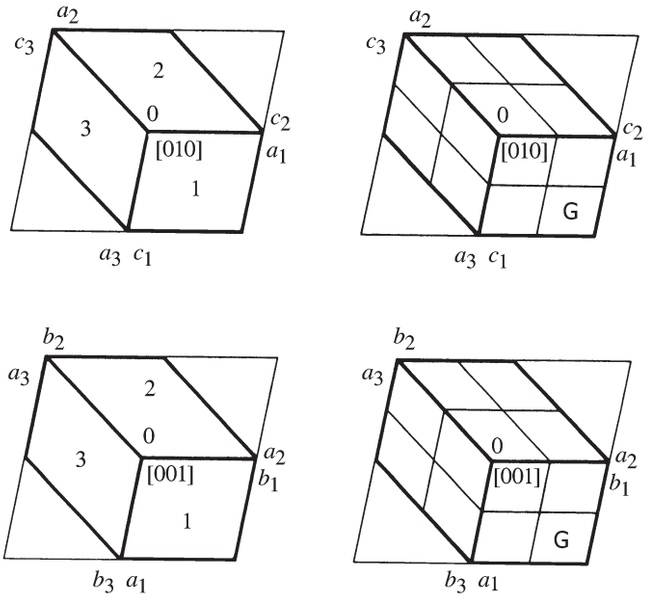


Figure 2.1.3.4
Monoclinic space groups, cell choices 1, 2, 3. Upper pair of diagrams: setting with unique axis *b*. Lower pair of diagrams: setting with unique axis *c*. The numbers 1, 2, 3 within the cells and the subscripts of the labels of the axes indicate the cell choice (*cf.* Section 2.1.3.15). The unique axis points upwards from the page. G = general-position diagram.

2.1.3.6.4. Orthorhombic space groups and orthorhombic settings

The space-group tables contain a set of four diagrams for each orthorhombic space group. The set consists of three projections of the symmetry elements [along the *c* axis (upper left), the *a* axis (lower left) and the *b* axis (upper right)] in addition to the general-position diagram, which is given only in the projection along *c* (lower right). The projected axes, the origins and the projection directions of these diagrams are illustrated in Fig. 2.1.3.5. They refer to the so-called 'standard setting' of the space group, *i.e.* the setting described in the space-group tables and indicated by the 'standard Hermann–Mauguin symbol' in the headline.

For each orthorhombic space group, *six settings* exist, *i.e.* six different ways of assigning the labels *a*, *b*, *c* to the three orthorhombic symmetry directions; thus the shape and orientation of the cell are the same for each setting. These settings correspond

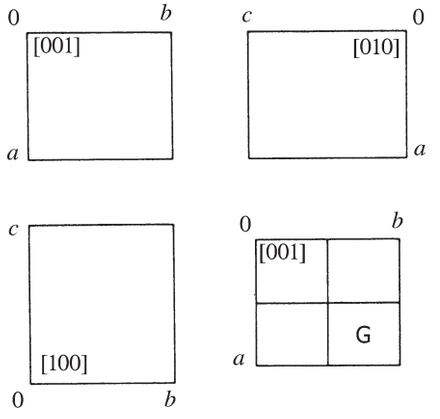


Figure 2.1.3.5
Orthorhombic space groups. Diagrams for the 'standard setting' as described in the space-group tables (G = general-position diagram).

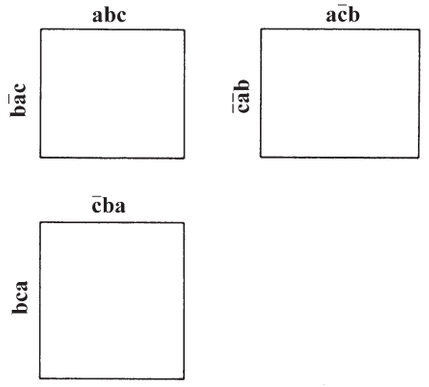


Figure 2.1.3.6
Orthorhombic space groups. The three projections of the symmetry elements with the six setting symbols (see text). For setting symbols printed vertically, the page has to be turned clockwise by 90° or viewed from the side. Note that in the actual space-group tables instead of the setting symbols the corresponding full Hermann–Mauguin space-group symbols are printed.

to the six permutations of the labels of the axes (including the identity permutation); *cf.* Section 1.5.4.3:

$$\mathbf{abc} \quad \mathbf{ba\bar{c}} \quad \mathbf{cab} \quad \mathbf{\bar{c}ba} \quad \mathbf{bca} \quad \mathbf{a\bar{c}b}.$$

The symbol for each setting, here called 'setting symbol', is a shorthand notation for the (3×3) transformation matrix $\boldsymbol{P}$ of the basis vectors of the standard setting, **a**, **b**, **c**, into those of the setting considered (*cf.* Chapter 1.5 for a detailed discussion of coordinate transformations). For instance, the setting symbol **cab** stands for the cyclic permutation

$$\mathbf{a}' = \mathbf{c}, \quad \mathbf{b}' = \mathbf{a}, \quad \mathbf{c}' = \mathbf{b}$$

or

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\,\boldsymbol{P} = (\mathbf{a}, \mathbf{b}, \mathbf{c})\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (\mathbf{c}, \mathbf{a}, \mathbf{b}),$$

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. An interchange of two axes reverses the handedness of the coordinate system; in order to keep the system right-handed, each interchange is accompanied by the reversal of the sense of one axis, *i.e.* by an element $\bar{1}$ in the transformation matrix. Thus, **ba$\bar{\mathbf{c}}$** denotes the transformation

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} = (\mathbf{b}, \mathbf{a}, \bar{\mathbf{c}}).$$

The six orthorhombic settings correspond to six Hermann–Mauguin symbols which, however, need not all be different; *cf.* Table 2.1.3.4.[1]

In the earlier (1935 and 1952) editions of *International Tables*, only one setting was illustrated, in a projection along **c**, so that it was usual to consider it as the 'standard setting' and to accept its cell edges as crystal axes and its space-group symbol as the 'standard Hermann–Mauguin symbol'. In the present edition, following *IT* A (2002), however, *all six* orthorhombic settings are illustrated, as explained below.

The three projections of the symmetry elements can be interpreted in two ways. First, in the sense indicated above, that is, as different projections of a *single* (standard) setting of the space group, with the projected basis vectors **a**, **b**, **c** labelled as in Fig. 2.1.3.5. Second, each one of the three diagrams can be considered as the projection along $\mathbf{c}'$ of either one of *two different* settings: one setting in which $\mathbf{b}'$ is horizontal and one in which $\mathbf{b}'$ is vertical ($\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ refer to the setting under consideration). This second interpretation is used to illustrate in the same figure the space-group symbols corresponding to these two settings. In order to view these projections in conventional orientation ($\mathbf{b}'$ horizontal, $\mathbf{a}'$ vertical, origin in the upper left corner, projection down the positive $\mathbf{c}'$ axis), the setting with $\mathbf{b}'$ horizontal can be inspected directly with the figure upright; hence, the corresponding space-group symbol is printed above the projection. The other setting with $\mathbf{b}'$ vertical and $\mathbf{a}'$ horizontal, however, requires turning the figure by 90°, or looking at it from the side; thus, the space-group symbol is printed at the left, and it runs upwards.

The 'setting symbols' for the six settings are attached to the three diagrams of Fig. 2.1.3.6, which correspond to those of Fig. 2.1.3.5. In the orientation of the diagram where the setting symbol is read in the usual way, $\mathbf{a}'$ is vertical pointing downwards, $\mathbf{b}'$ is horizontal pointing to the right, and $\mathbf{c}'$ is pointing upwards from the page. Each setting symbol is printed in the position that in the space-group tables is actually occupied by the corresponding full Hermann–Mauguin symbol. The changes in the space-group symbol that are associated with a particular setting

Table 2.1.3.4
Numbers of distinct projections and different Hermann–Mauguin symbols for the orthorhombic space groups

The space-group numbers are given in parentheses. The space groups are listed according to point group as indicated in the column headings.

Number of distinct projections	222	*mm*2	2/*m* 2/*m* 2/*m*
6 (22 space groups)		*Pmc*2_1 (26) *Pma*2 (28) *Pca*2_1 (29) *Pnc*2 (30) *Pna*2_1 (33) *Cmc*2_1 (36) *Amm*2 (38) *Aem*2 (39) *Ama*2 (40) *Aea*2 (41) *Ima*2 (46)	*P* $2_1/m$ 2/*m* 2/*a* (51) *P* 2/*n* $2_1/n$ 2/*a* (52) *P* 2/*m* 2/*n* $2_1/a$ (53) *P* $2_1/c$ 2/*c* 2/*a* (54) *Pmn*2_1 (31) *P* 2/*b* $2_1/c$ $2_1/m$ (57) *P* $2_1/b$ 2/*c* $2_1/n$ (60) *P* $2_1/n$ $2_1/m$ $2_1/a$ (62) *C* 2/*m* 2/*c* $2_1/m$ (63) *C* 2/*m* 2/*c* $2_1/e$ (64) *I* $2_1/m$ $2_1/m$ $2_1/a$ (74)
3 (25 space groups)	*P*222$_1$ (17) *P*2_12_12 (18) *C*222$_1$ (20) *C*222 (21)	*Pmm*2 (25) *Pcc*2 (27) *Pba*2 (32) *Pnn*2 (34) *Cmm*2 (35) *Ccc*2 (37) *Fmm*2 (42) *Fdd*2 (43) *Imm*2 (44) *Iba*2 (45)	*P* 2/*c* 2/*c* 2/*m* (49) *P* 2/*b* 2/*a* 2/*n* (50) *P* $2_1/b$ $2_1/a$ 2/*m* (55) *P* $2_1/c$ $2_1/c$ 2/*n* (56) *P* $2_1/n$ $2_1/n$ 2/*m* (58) *P* $2_1/m$ $2_1/m$ 2/*n* (59) *C* 2/*m* 2/*m* 2/*m* (65) *C* 2/*c* 2/*c* 2/*m* (66) *C* 2/*m* 2/*m* 2/*e* (67) *C* 2/*c* 2/*c* 2/*e* (68) *I* 2/*b* 2/*a* 2/*m* (72)
2 (2 space groups)			*P* $2_1/b$ $2_1/c$ $2_1/a$ (61) *I* $2_1/b$ $2_1/c$ $2_1/a$ (73)
1 (10 space groups)	*P*222 (16) *P*$2_12_12_1$ (19) *F*222 (22) *I*222 (23) *I*$2_12_12_1$ (24)		*P* 2/*m* 2/*m* 2/*m* (47) *P* 2/*n* 2/*n* 2/*n* (48) *F* 2/*m* 2/*m* 2/*m* (69) *F* 2/*d* 2/*d* 2/*d* (70) *I* 2/*m* 2/*m* 2/*m* (71)
Total: 59	9	22	28

[1] A space-group symbol is invariant under sign changes of the axes; *i.e.* the same symbol applies to the right-handed coordinate systems **abc**, **ab$\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}$b$\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}\bar{\mathbf{b}}$c** and the left-handed systems **$\bar{\mathbf{a}}\bar{\mathbf{b}}\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}$bc**, **ab$\bar{\mathbf{c}}$**, **$\bar{\mathbf{a}}\bar{\mathbf{b}}$c**.

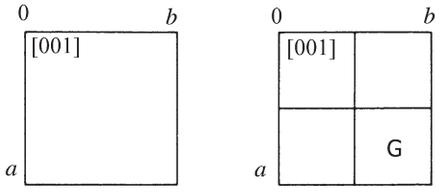


Figure 2.1.3.7
Tetragonal space groups (G = general-position diagram).

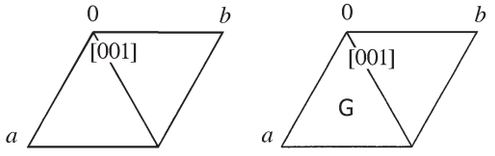


Figure 2.1.3.8
Trigonal *P* and hexagonal *P* space groups (G = general-position diagram).

symbol can easily be deduced by comparing Fig. 2.1.3.6 with the diagrams for the space group under consideration.

Not all of the 59 orthorhombic space groups have all six projections distinct, *i.e.* have different Hermann–Mauguin symbols for the six settings. This aspect is treated in Table 2.1.3.4. Only 22 space groups have six, 25 have three, 2 have two different symbols, while 10 have all symbols the same. This information can be of help in the early stages of a crystal-structure analysis.

The six setting symbols, *i.e.* the six permutations of the labels of the axes, form the column headings of the orthorhombic entries in Table 1.5.4.4, which contains the extended Hermann–Mauguin symbols for the six settings of each orthorhombic space group. Note that some of these setting symbols exhibit different sign changes compared with those in Fig. 2.1.3.6.

2.1.3.6.5. Tetragonal, trigonal P and hexagonal P space groups

The pairs of diagrams for these space groups are similar to those in the previous editions of *IT*. Each pair consists of a general-position diagram (right) and a diagram of the symmetry elements (left), both projected along **c**, as illustrated in Figs. 2.1.3.7 and 2.1.3.8.

2.1.3.6.6. Trigonal R (rhombohedral) space groups

The seven rhombohedral space groups are treated in two versions, the first based on 'hexagonal axes' (obverse setting), the second on 'rhombohedral axes' (*cf.* Sections 2.1.1.2 and 2.1.3.2). The pairs of diagrams are similar to those in *IT* (1952) and *IT* A (2002); the left or top one displays the symmetry elements, the right or bottom one the general position. This is illustrated in Fig. 2.1.3.9, which gives the axes *a* and *b* of the triple hexagonal cell and the projections of the axes of the primitive rhombohedral cell, labelled $a_{\rm rh}$, $b_{\rm rh}$ and $c_{\rm rh}$. For convenience, all 'heights' in the space-group diagrams are fractions of the hexagonal *c* axis. For 'hexagonal axes', the projection direction is [001], for 'rhombohedral axes' it is [111]. In the general-position diagrams, the circles drawn in heavier lines represent atoms that lie within the primitive rhombohedral cell (provided the symbol '—' is read as $1 - z$ rather than as $-z$).

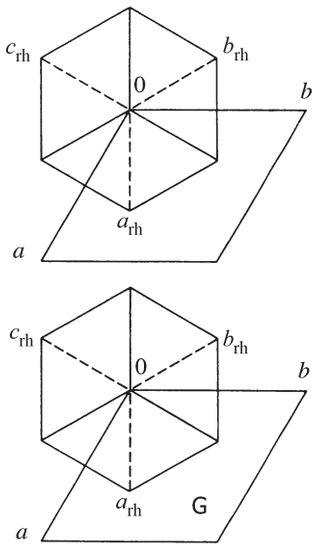


Figure 2.1.3.9
Rhombohedral space groups. Obverse triple hexagonal cell with 'hexagonal axes' *a*, *b* and primitive rhombohedral cell with projections of 'rhombohedral axes' $a_{\rm rh}$, $b_{\rm rh}$, $c_{\rm rh}$. Note: In the actual space-group diagrams the edges of the primitive rhombohedral cell (dashed lines) are only indicated in the general-position diagram of the rhombohedral-axes description (G = general-position diagram).

The symmetry-element diagrams for the hexagonal and the rhombohedral descriptions of a space group are the same. The edges of the primitive rhombohedral cell (*cf.* Fig. 2.1.3.9) are only indicated in the general-position diagram of the rhombohedral description.

2.1.3.6.7. Cubic space groups

For each cubic space group, one projection of the symmetry elements along [001] is given, Fig. 2.1.3.10; for details of the diagrams, see Section 2.1.2 and Buerger (1956). For face-centred lattices *F*, only a quarter of the unit cell is shown; this is sufficient since the projected arrangement of the symmetry elements is translation-equivalent in the four quarters of an *F* cell. It is important to note that symmetry axes inclined to the projection plane are indicated where they intersect the plane of projection. Symmetry planes inclined to the projection plane that occur in classes $\bar{4}3m$ and $m\bar{3}m$ are shown as 'inserts' around the high-symmetry points, such as 0, 0, 0; $\frac{1}{2}$, 0, 0; *etc.*

The cubic diagrams given in *IT* (1935) are different from the ones used here. No drawings for cubic space groups were provided in *IT* (1952).

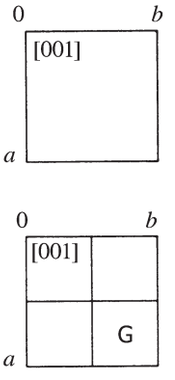


Figure 2.1.3.10
Cubic space groups. G = general-position diagram, in which the equivalent positions are shown as the vertices of polyhedra.

2.1.3.6.8. Diagrams of the general position (by K. Momma and M. I. Aroyo)

Non-cubic space groups. In these diagrams, the 'heights' of the points are z coordinates, except for monoclinic space groups with unique axis b where they are y coordinates. For rhombohedral space groups, the heights are always fractions of the hexagonal c axis. The symbols + and − stand for $+z$ and $-z$ (or $+y$ and $-y$) in which z or y can assume any value. For points with symbols + or − preceded by a fraction, *e.g.* $\frac{1}{2}+$ or $\frac{1}{3}-$, the relative z or y coordinate is $\frac{1}{2}$ *etc.* higher than that of the point with symbol + or −.

Where a mirror plane exists parallel to the plane of projection, the two positions superimposed in projection are indicated by the use of a ring divided through the centre. The information given on each side refers to one of the two positions related by the mirror plane, as in $-$ ⏀ $+$.

Diagrams for cubic space groups (Fig. 2.1.3.10). Following the approach of *IT* (1935), for each cubic space group a diagram showing the points of the general position as the vertices of polyhedra is given. In these diagrams, the polyhedra are transparent, but the spheres at the vertices are opaque. For most of the space groups, 'starting points' with the same coordinate values, $x = 0.048$, $y = 0.12$, $z = 0.089$, have been used. The origins of the polyhedra are chosen at special points of highest site symmetry, which for most space groups coincide with the origin (and its equivalent points in the unit cell). Polyhedra with origins at sites $(\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$ have been chosen for the space groups $P4_332$ (212) and $I4_132$ (214), and $(\frac{3}{8}, \frac{3}{8}, \frac{3}{8})$ for $P4_132$ (213). The two diagrams shown for the space groups $I\bar{4}3d$ (220) and $Ia\bar{3}d$ (230) correspond to polyhedra with origins chosen at two different special sites with site-symmetry groups of equal (32 *versus* $\bar{3}$ in $Ia\bar{3}d$) or nearly equal order (3 *versus* $\bar{4}$ in $I\bar{4}3d$). The height h of the centre of each polyhedron is given on the diagram, if different from zero. For space-group Nos. 198, 199 and 220, h refers to the special point to which the polyhedron (triangle) is connected. Polyhedra with height 1 are omitted in all the diagrams. A grid of four squares is drawn to represent the four quarters of the basal plane of the cell. For space groups $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226) and $Fd\bar{3}c$ (228), where the number of points is too large for one diagram, two diagrams are provided, one for the upper half and one for the lower half of the cell.

Notes:

(i) For space group $P4_132$ (213), the coordinates $\bar{x}, \bar{y}, \bar{z}$ have been chosen for the 'starting point' to show the enantiomorphism with $P4_332$ (212).

(ii) For the description of a space group with 'origin choice 2', the coordinates x, y, z of all points have been shifted with the origin to retain the same polyhedra for both origin choices.

An additional general-position diagram is shown on the fourth page for each of the ten space groups of the $m\bar{3}m$ crystal class. To provide a clearer three-dimensional-style overview of the arrangements of the polyhedra, these general-position diagrams are shown in tilted projection (in contrast to the orthogonal-projection diagrams described above).

The general-position diagrams of the cubic groups in both orthogonal and tilted projections were generated using the program *VESTA* (Momma & Izumi, 2011).

Readers who wish to compare other approaches to space-group diagrams and their history are referred to *IT* (1935), *IT* (1952), the fifth edition of *IT* A (2002) (where general-position stereodiagrams of the cubic space groups are shown) and the following publications: Astbury & Yardley (1924), Belov *et al.* (1980), Buerger (1956), Fedorov (1895; English translation, 1971), Friedel (1926), Hilton (1903), Niggli (1919) and Schiebold (1929).

2.1.3.7. Origin

The determination and description of crystal structures and particularly the application of direct methods are greatly facilitated by the choice of a suitable origin and its proper identification. This is even more important if related structures are to be compared or if 'chains' of group–subgroup relations are to be constructed. In this volume, as well as in *IT* (1952) and *IT* A (2002), the origin of the unit cell has been chosen according to the following conventions (*cf.* Sections 2.1.1 and 2.1.3.2):

(i) All centrosymmetric space groups are described with an inversion centre as origin. A further description is given if a centrosymmetric space group contains points of high site symmetry that do not coincide with a centre of symmetry. As an example, study the origin choice 1 and origin choice 2 descriptions of $I4_1/amd$ (141).

(ii) For noncentrosymmetric space groups, the origin is at a point of highest site symmetry, as in $P\bar{6}m2$ (187). If no site symmetry is higher than 1, except for the cases listed below under (iii), the origin is placed on a screw axis, or a glide plane, or at the intersection of several such symmetry elements, see for example space groups $Pca2_1$ (29) and $P6_1$ (169).

(iii) In space group $P2_12_12_1$ (19), the origin is chosen in such a way that it is surrounded symmetrically by three pairs of 2_1 axes. This principle is maintained in the following noncentrosymmetric cubic space groups of classes 23 and 432, which contain $P2_12_12_1$ as subgroup: $P2_13$ (198), $I2_13$ (199), $F4_132$ (210). It has been extended to other noncentrosymmetric orthorhombic and cubic space groups with $P2_12_12_1$ as subgroup, even though in these cases points of higher site symmetry *are* available: $I2_12_12_1$ (24), $P4_332$ (212), $P4_132$ (213), $I4_132$ (214).

There are several ways of determining the location and site symmetry of the origin. First, the origin can be inspected directly in the space-group diagrams (*cf.* Section 2.1.3.6). This method permits visualization of all symmetry elements that intersect the chosen origin.

Another procedure for finding the site symmetry at the origin is to look for a special position that contains the coordinate triplet 0, 0, 0 or that includes it for special values of the parameters, *e.g.* position 1*a:* 0, 0, z in space group $P4$ (75), or position 3*a*: $x, 0, \frac{1}{3}$; $0, x, \frac{2}{3}$; $\bar{x}, \bar{x}, 0$ in space group $P3_121$ (152). If such a special position occurs, the symmetry at the origin is given by the oriented site-symmetry symbol (see Section 2.1.3.12) of that special position; if it does not occur, the site symmetry at the origin is 1. For most practical purposes, these two methods are sufficient for the identification of the site symmetry at the origin.

Origin statement. In the line *Origin* immediately below the diagrams, the site symmetry of the origin is stated, if different from the identity. A further symbol indicates all symmetry elements (including glide planes and screw axes) that pass through the origin, if any. For space groups with two *origin choices*, for each of the two origins the location relative to the other origin is also given. An example is space group *Ccce* (68).

In order to keep the notation as simple as possible, no rigid rules have been applied in formulating the origin statements. Their meaning is demonstrated by the examples in Table 2.1.3.5,

Table 2.1.3.5
Examples of origin statements

Example number	Space group (No.)	Origin statement	Meaning of last symbol in *E*4–*E*11
*E*1	$P\bar{1}$ (2)	at $\bar{1}$	
*E*2	$P2/m$ (10)	at centre $(2/m)$	
*E*3	*P*222 (16)	at $\bar{2}\bar{2}\bar{2}$	
*E*4	*Pcca* (54)	at $\bar{1}$ on 1*ca*	$c \perp [010]$, $a \perp [001]$
*E*5	*Cmcm* (63)	at centre $(2/m)$ at $2/mc2_1$	$2 \parallel [100]$, $m \perp [100]$, $c \perp [010]$, $2_1 \parallel [001]$
*E*6	*Pcc*2 (27)	on *cc*2; short for: on 2 on *cc*2	$c \perp [100]$, $c \perp [010]$, $2 \parallel [001]$
*E*7	*P*4*bm* (100)	on 41*g*; short for: on 4 on 41*g*	$4 \parallel [001]$, $g \perp [1\bar{1}0]$ and $g \perp [110]$
*E*8	$P4_2mc$ (105)	on 2*mm* on 4_2mc	$4_2 \parallel [001]$, $m \perp [100]$ and $m \perp [010]$, $c \perp [1\bar{1}0]$ and $c \perp [110]$
*E*9	$P4_32_12$ (96)	on 2[110] at $2_11(1, 2)$	$2_1 \parallel [001]$, 1 in $[1\bar{1}0]$ and $2 \parallel [110]$
*E*10	$P3_121$ (152)	on 2[110] at $3_1(1, 1, 2)1$	$3_1 \parallel [001]$, $2 \parallel [110]$
*E*11	$P3_112$ (151)	on 2[210] at $3_11(1, 1, 2)$	$3_1 \parallel [001]$, $2 \parallel [210]$

which should be studied together with the appropriate space-group diagrams.

These examples illustrate the following points:

(i) The site symmetry at the origin corresponds to the point group of the space group (examples *E*1–*E*3) or to a subgroup of this point group (*E*4–*E*11).

The presence of a symmetry centre at the origin is always stated explicitly, either by giving the symbol $\bar{1}$ (*E*1 and *E*4) or by the words 'at centre', followed by the full site symmetry between parentheses (*E*2 and *E*5). This completes the origin line if no further glide planes or screw axes are present at the origin.

(ii) If glide planes or screw axes are present, as in examples *E*4–*E*11, they are given in the order of the symmetry directions listed in Table 2.1.3.1. Such a set of symmetry elements is described here in the form of a 'point-group-like' symbol (although it does not describe a group). With the help of the orthorhombic symmetry directions, the symbols in *E*4–*E*6 can be interpreted easily. The shortened notation of *E*6 and *E*7 is used for space groups of crystal classes *mm*2, 4*mm*, $\bar{4}2m$, 3*m*, 6*mm* and $\bar{6}2m$ if the site symmetry at the origin can be easily recognized from the shortened symbol.

(iii) For the tetragonal, trigonal and hexagonal space groups, the situation is more complicated than for the orthorhombic groups. The tetragonal space groups have one primary, two secondary and two tertiary symmetry directions. For hexagonal groups, these numbers are one, three and three (Table 2.1.3.1). If the symmetry elements passing through the origin are the same for the two (three) secondary or the two (three) tertiary directions, only one entry is given at the relevant position of the origin statement [example *E*7: 'on 41*g*' instead of 'on 41(*g*, *g*)']. An exception occurs for the site-symmetry group 2*mm* (example *E*8), which is always written in full rather than as 2*m*1.

If the symmetry elements are different, two (three) symbols are placed between parentheses, which stand for the two (three) secondary or tertiary directions. The order of these symbols corresponds to the order of the symmetry directions within the secondary or tertiary set, as listed in Table 2.1.3.1. Directions without symmetry are indicated by the symbol 1. With this rule, the last symbols in the examples *E*9–*E*11 can be interpreted.

Note that for some tetragonal space groups (Nos. 100, 113, 125, 127, 129, 134, 138, 141, 142) the glide-plane symbol *g* is used in the origin statement. This symbol occurs also in the block *Symmetry operations* of these space groups; it is explained in Sections 2.1.3.9 and 1.4.2.1.

(iv) To emphasize the orientation of the site-symmetry elements at the origin, examples *E*9 and *E*10 start with 'on 2[110]' and *E*11 with 'on 2[210]'. In *E*8, the site-symmetry group is 2*mm*. Together with the space-group symbol this indicates that 2 is along the primary tetragonal direction, that the two symbols *m* refer to the two secondary symmetry directions [100] and [010], and that the tertiary set of directions does not contribute to the site symmetry.

For monoclinic space groups, an indication of the orientation of the symmetry elements is not necessary; hence, the site symmetry at the origin is given by non-oriented symbols. For orthorhombic space groups, the orientation is obvious from the symbol of the space group.

(v) The extensive description of the symmetry elements passing through the origin is not retained for the cubic space groups, as this would have led to very complicated notations for some of the groups.

2.1.3.8. Asymmetric unit

An asymmetric unit of a space group is a (simply connected) smallest closed part of space from which, by application of all symmetry operations of the space group, the whole of space is filled. This implies that mirror planes and rotation axes must form boundary planes and boundary edges of the asymmetric unit. A twofold rotation axis may bisect a boundary plane. Centres of inversion must either form vertices of the asymmetric unit or be located at the midpoints of boundary planes or boundary edges. For glide planes and screw axes, these simple restrictions do not hold. An asymmetric unit contains all the information necessary for the complete description of the crystal structure. In mathematics, an asymmetric unit is called 'fundamental region' or 'fundamental domain'.

Example

The boundary planes of the asymmetric unit in space group *Pmmm* (47) are fixed by the six mirror planes $x, y, 0$; $x, y, \frac{1}{2}$; $x, 0, z$; $x, \frac{1}{2}, z$; $0, y, z$; and $\frac{1}{2}, y, z$. For space group $P2_12_12_1$ (19), on the other hand, a large number of connected regions, each with a volume of $\frac{1}{4}V$(cell), may be chosen as asymmetric unit.

In cases where the asymmetric unit is not uniquely determined by symmetry, its choice may depend on the purpose of its application. For the description of the structures of molecular crystals, for instance, it is advantageous to select asymmetric units that contain one or more complete molecules. In the space-group tables of this volume, following *IT* A (2002), the asymmetric units

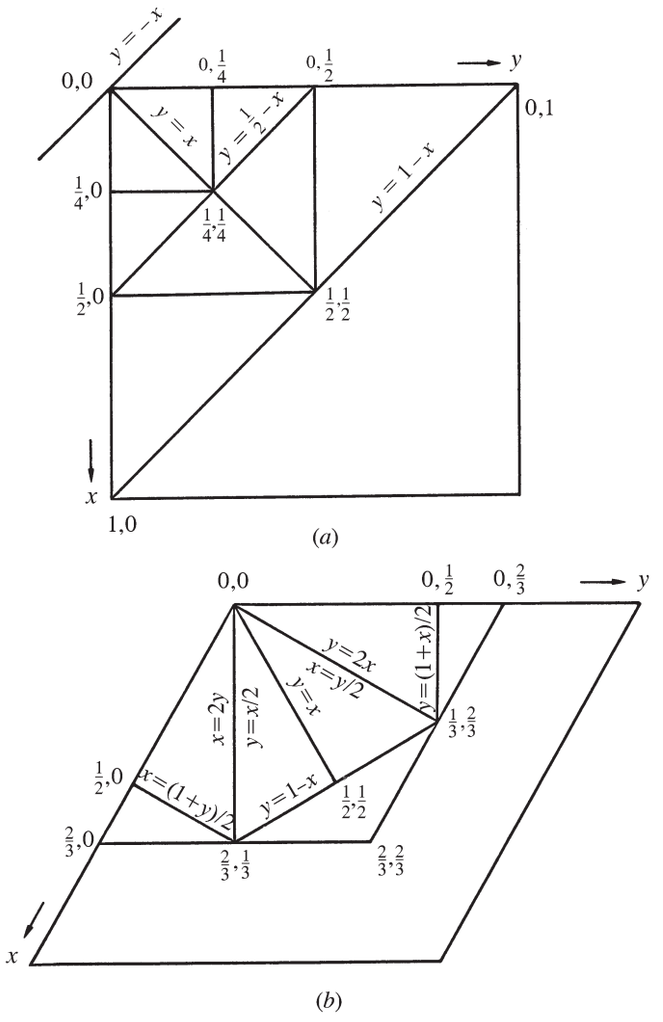


Figure 2.1.3.11
Boundary planes of asymmetric units occurring in the space-group tables. (*a*) Tetragonal system. (*b*) Trigonal and hexagonal systems. The point coordinates refer to the vertices in the plane $z = 0$.

are chosen in such a way that Fourier summations can be performed conveniently.

For all triclinic, monoclinic and orthorhombic space groups, the asymmetric unit is chosen as a parallelepiped with one vertex at the origin of the cell and with boundary planes parallel to the faces of the cell. It is given by the notation

$$0 \le x_i \le \text{upper limit of } x_i,$$

where x_i stands for x, y or z.

For space groups with higher symmetry, cases occur where the origin does not coincide with a vertex of the asymmetric unit or where not all boundary planes of the asymmetric unit are parallel to those of the cell. In all these cases, parallelepipeds

$$\text{lower limit of } x_i \le x_i \le \text{upper limit of } x_i$$

are given that are equal to or larger than the asymmetric unit. Where necessary, the boundary planes lying within these parallelepipeds are given by additional inequalities, such as $x \le y$, $y \le \frac{1}{2} - x$ *etc.*

In the trigonal, hexagonal and especially the cubic crystal systems, the asymmetric units have complicated shapes. For this reason, they are also specified by the coordinates of their vertices. Drawings of asymmetric units for cubic space groups have been published by Koch & Fischer (1974). Fig. 2.1.3.11 shows the boundary planes occurring in the tetragonal, trigonal and hexagonal systems, together with their algebraic equations.

Examples

(1) In space group *P*4*mm* (99), the boundary plane $y = x$ occurs in addition to planes parallel to the unit-cell faces; the asymmetric unit is given by

$$0 \le x \le \tfrac{1}{2}; \quad 0 \le y \le \tfrac{1}{2}; \quad 0 \le z \le 1; \quad x \le y.$$

(2) In *P*4*bm* (100), one of the boundary planes is $y = \frac{1}{2} - x$. The asymmetric unit is given by

$$0 \le x \le \tfrac{1}{2}; \quad 0 \le y \le \tfrac{1}{2}; \quad 0 \le z \le 1; \quad y \le \tfrac{1}{2} - x.$$

(3) In space group *R*32 (155; hexagonal axes), the boundary planes are, among others, $x = (1 + y)/2$, $y = 1 - x$, $y = (1 + x)/2$. The asymmetric unit is defined by

$$0 \le x \le \tfrac{2}{3}; \quad 0 \le y \le \tfrac{2}{3}; \quad 0 \le z \le \tfrac{1}{6};$$
$$x \le (1 + y)/2; \quad y \le \min(1 - x, (1 + x)/2)$$

Vertices: $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{6}$ $\frac{1}{2},0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ $0,\frac{1}{2},\frac{1}{6}$.

It is obvious that the indication of the vertices is of great help in drawing the asymmetric unit.

Fourier syntheses. For complicated space groups, the easiest way to calculate Fourier syntheses is to consider the parallelepiped listed, without taking into account the additional boundary planes of the asymmetric unit. These planes should be drawn afterwards in the Fourier synthesis. For the computation of integrated properties from Fourier syntheses, such as the number of electrons for parts of the structure, the values at the boundaries of the asymmetric unit must be applied with a reduced weight if the property is to be obtained as the product of the content of the asymmetric unit and the multiplicity.

Example

In the parallelepiped of space group *Pmmm* (47), the weights for boundary planes, edges and vertices are $\frac{1}{2}$, $\frac{1}{4}$ and $\frac{1}{8}$, respectively.

Asymmetric units of the plane groups have been discussed by Buerger (1949, 1960) in connection with Fourier summations.

2.1.3.9. Symmetry operations

As explained in Sections 1.3.3.2 and 1.4.2.3, the coordinate triplets of the *General position* of a space group may be interpreted as a shorthand description of the symmetry operations in matrix notation. The geometric description of the symmetry operations is found in the space-group tables under the heading *Symmetry operations*.

Numbering scheme. The numbering (1) . . . (*p*) . . . of the entries in the blocks *Symmetry operations* and *General position* (first block below *Positions*) is the same. Each listed coordinate triplet of the general position is preceded by a number between parentheses (*p*). The same number (*p*) precedes the corresponding symmetry operation. For space groups with *primitive* cells, the two lists contain the same number of entries.

For space groups with *centred* cells, several (2, 3 or 4) blocks of *Symmetry operations* correspond to the one *General position* block. The numbering scheme of the general position is applied to each one of these blocks. The number of blocks equals the multiplicity of the centred cell, *i.e.* the number of centring translations below the subheading *Coordinates*, such as $(0,0,0)+$, $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$, $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$.

Whereas for the *Positions* the reader is expected to add these centring translations to each printed coordinate triplet themselves (in order to obtain the complete general position), for the *Symmetry operations* the corresponding data are listed explicitly. The different blocks have the subheadings 'For $(0,0,0)+$ set', 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set', *etc.* Thus, an obvious one-to-one correspondence exists between the analytical description of a symmetry operation in the form of its general-position coordinate triplet and the geometrical description under *Symmetry operations*. Note that the coordinates are reduced modulo 1, where applicable, as shown in the example below.

Example: Ibca (73)

The centring translation is $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Accordingly, above the general position one finds $(0,0,0)+$ and $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$. In the block *Symmetry operations*, under the subheading 'For $(0,0,0)+$ set', entry (2) refers to the coordinate triplet $\bar{x}+\frac{1}{2}$, $\bar{y}$, $z+\frac{1}{2}$. Under the subheading 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set', however, entry (2) refers to $\bar{x}$, $\bar{y}+\frac{1}{2}$, z. The triplet $\bar{x}$, $\bar{y}+\frac{1}{2}$, z is selected rather than $\bar{x}+1$, $\bar{y}+\frac{1}{2}$, $z+1$, because the coordinates are reduced modulo 1.

The coordinate triplets of the general position represent the symmetry operations chosen as coset representatives of the decomposition of the space group with respect to its translation subgroup (*cf.* Section 1.4.2 for a detailed discussion). In space groups with two origins the origin shift may lead to the choice of symmetry operations of different types as coset representatives of the same coset (*e.g.* mirror *versus* glide plane, rotation *versus* screw axis, see Tables 1.4.2.2 and 1.4.2.3) and designated by the same number (p) in the general-position blocks of the two descriptions. Thus, in $P4/nmm$ (129), (p) = (7) represents a 2 and a 2_1 axis, both in $x, x, 0$, whereas (p) = (16) represents a g and an m plane, both in x, x, z.

Designation of symmetry operations. An entry in the block *Symmetry operations* is characterized as follows.

(i) A symbol denoting the *type* of the symmetry operation (*cf.* Section 2.1.2), including its glide or screw part, if present. In most cases, the glide or screw part is given explicitly by fractional coordinates between parentheses. The sense of a rotation is indicated by the superscript + or −. Abbreviated notations are used for the glide reflections $a(\frac{1}{2},0,0)\equiv a$; $b(0,\frac{1}{2},0)\equiv b$; $c(0,0,\frac{1}{2})\equiv c$. Glide reflections with complicated and unconventional glide parts are designated by the letter g, followed by the glide part between parentheses.

(ii) A coordinate triplet indicating the *location* and *orientation* of the symmetry element which corresponds to the symmetry operation. For rotoinversions, the location of the inversion point is also given.

Examples

(1) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $\quad x, x, z$
Glide reflection with glide component $(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ through the plane x, x, z, *i.e.* the plane parallel to $(1\bar{1}0)$ containing the point 0, 0, 0.

(2) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ $\quad 2x-\frac{1}{2}, x, z$ (hexagonal axes)
Glide reflection with glide component $(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ through the plane $2x-\frac{1}{2}, x, z$, *i.e.* the plane parallel to $(1\bar{2}10)$, which intersects the a axis at $-\frac{1}{2}$ and the b axis at $\frac{1}{4}$; this operation occurs in $R\bar{3}c$ (167, hexagonal axes).

(3) Symmetry operations in *Ibca* (73)
Under the subheading 'For $(0,0,0)+$ set', the operation generating the coordinate triplet (2) $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$ from (1) x, y, z is symbolized by $2(0,0,\frac{1}{2})$ $\frac{1}{4}, 0, z$. This indicates a twofold screw rotation with screw part $(0,0,\frac{1}{2})$ for which the corresponding screw axis coincides with the line $\frac{1}{4}, 0, z$, *i.e.* runs parallel to [001] through the point $\frac{1}{4}, 0, 0$. Under the subheading 'For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set', the operation generating the coordinate triplet (2) $\bar{x}, \bar{y}+\frac{1}{2}, z$ from (1) x, y, z is symbolized by $2\ 0,\frac{1}{4}, z$. It is thus a twofold rotation (without screw part) around the line $0,\frac{1}{4}, z$.

Details on the symbolism and further illustrative examples are presented in Section 1.4.2.1.

2.1.3.10. Generators

The line *Generators selected* states the symmetry operations and their sequence, selected to generate all symmetry-equivalent points of the *General position* from a point with coordinates x, y, z. Generating translations are listed as $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$; likewise for additional centring translations. The other symmetry operations are given as numbers (p) that refer to the corresponding coordinate triplets of the general position and the corresponding entries under *Symmetry operations*, as explained in Section 2.1.3.9 [for centred space groups the first block 'For $(0,0,0)+$ set' must be used].

For all space groups, the identity operation given by (1) is selected as the first generator. It is followed by the generators $t(1,0,0)$, $t(0,1,0)$, $t(0,0,1)$ of the integral lattice translations and, if necessary, by those of the centring translations, *e.g.* $t(\frac{1}{2},\frac{1}{2},0)$ for a C-centred lattice. In this way, point *x, y, z* and all its translationally equivalent points are generated. (The remark 'and its translationally equivalent points' will hereafter be omitted.) The sequence chosen for the generators following the translations depends on the crystal class of the space group and is set out in Table 1.4.3.1.

Example: $P12_1/c1$ (14, unique axis b, cell choice 1)

After the generation of (1) x, y, z, the operation (2) which stands for a twofold screw rotation around the axis $0, y, \frac{1}{4}$ generates point (2) of the general position with coordinate triplet $\bar{x}, y+\frac{1}{2}, \bar{z}+\frac{1}{2}$. Finally, the inversion (3) generates point (3) $\bar{x}, \bar{y}, \bar{z}$ from point (1), and point (4′) $x, \bar{y}-\frac{1}{2}, z-\frac{1}{2}$ from point (2). Instead of (4′), however, the coordinate triplet (4) $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$ is listed, because the coordinates are reduced modulo 1.

The example shows that for the space group $P12_1/c1$ two operations, apart from the identity and the generating translations, are sufficient to generate all symmetry-equivalent points. Alternatively, the inversion (3) plus the glide reflection (4), or the glide reflection (4) plus the twofold screw rotation (2), might have been chosen as generators. The process of generation and the selection of the generators for the space-group tables, as well as the resulting sequence of the symmetry operations, are discussed in Section 1.4.3.

The generating operations for different descriptions of the same space group (settings, cell choices, origin choices) are chosen in such a way that the transformation relating the two coordinate systems also transforms the generators of one description into those of the other (*cf.* Section 1.5.3).

2.1.3.11. Positions

The entries under *Positions*[2] (more explicitly called *Wyckoff positions*) consist of the one *General position* (upper block) and the *Special positions* (blocks below). The columns in each block, from left to right, contain the following information for each Wyckoff position.

(i) *Multiplicity of the Wyckoff position*. This is the number of equivalent points per unit cell. For primitive cells, the multiplicity of the general position is equal to the order of the point group of the space group; for centred cells, it is the product of the order of the point group and the number (2, 3 or 4) of lattice points per cell. The multiplicity of a special position is always a divisor of the multiplicity of the general position and the quotient of the two is equal to the order of the site-symmetry group.

(ii) *Wyckoff letter*. This letter is merely a coding scheme for the Wyckoff positions, starting with *a* at the bottom position and continuing upwards in alphabetical order.

(iii) *Site symmetry*. This is explained in Section 2.1.3.12.

(iv) *Coordinates*. The sequence of coordinate triplets is produced in the same order as the symmetry operations, generated by the chosen set of generators, omitting duplicates (*cf.* Sections 1.4.3 and 2.1.3.10). For centred space groups, the centring translations, for instance $(0,0,0)+\ (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$, are listed above the coordinate triplets. The symbol '+' indicates that, in order to obtain a complete Wyckoff position, the components of these centring translations have to be added to the listed coordinate triplets. Note that not all points of a position always lie within the unit cell; some may be outside since the coordinates are formulated modulo 1; thus, for example, $\bar{x}, \bar{y}, \bar{z}$ is written rather than $\bar{x}+1, \bar{y}+1, \bar{z}+1$.

The coordinate triplets of a position represent the coordinates of the equivalent points (atoms) in the unit cell. A graphic representation of the points of the general position is provided by the general-position diagram; *cf.* Section 2.1.3.6.

(v) *Reflection conditions*. These are described in Section 2.1.3.13.

Detailed treatment of general and special Wyckoff positions, including definitions, theoretical background and examples, is given in Section 1.4.4.

The two types of positions, general and special, are characterized as follows:

(i) *General position*

A point is said to be in general position if it is left invariant only by the identity operation but by no other symmetry operation of the space group. Each space group has only one general position.

The coordinate triplets of a general position (which always start with x, y, z) can also be interpreted as a shorthand form of the matrix representation of the symmetry operations of the space group; this viewpoint is described further in Sections 1.3.3.2 and 1.4.2.3.

(ii) *Special position(s)*

A point is said to be in 'special position' if it is mapped onto itself by the identity and at least one further symmetry operation of the space group. This implies that specific constraints are imposed on the coordinates of each point of a special position; *e.g.* $x=\frac{1}{4}, y=0$, leading to the triplet $\frac{1}{4}, 0, z$; or $y=x+\frac{1}{2}$, leading to the triplet $x, x+\frac{1}{2}, z$. The number of special positions of a space group depends on the space-group type and can vary from 1 to 26 (in *Pmmm*, No. 47).

The set of *all* symmetry operations that map a point onto itself forms a group, known as the 'site-symmetry group' of that point. It is given in the third column by the 'oriented site-symmetry symbol' which is explained in Section 2.1.3.12. General positions always have site symmetry 1, whereas special positions have higher site symmetries, which can differ from one special position to another.

If in a crystal structure the centres of finite objects, such as molecules, are placed at the points of a special position, each such object must display a point symmetry that is at least as high as the site symmetry of the special position. Geometrically, this means that the centres of these objects are located on symmetry elements without translations (centre of symmetry, mirror plane, rotation axis, rotoinversion axis) or at the intersection of several symmetry elements of this kind (*cf.* the space-group diagrams).

Note that the location of an object on a screw axis or on a glide plane does *not* lead to an increase in the site symmetry and to a corresponding reduction of the multiplicity for that object. Accordingly, a space group that contains only symmetry elements *with* translation components does not have any special position. Such a space group is called 'fixed-point-free' (for further discussion, see Section 1.4.4.2).

Example: Space group C12/c1 (15, unique axis b, cell choice 1)

The general position 8*f* of this space group contains eight equivalent points per cell, each with site symmetry 1. The coordinate triplets of four points, (1) to (4), are given explicitly, the coordinates of the other four points are obtained by adding the components $\frac{1}{2}, \frac{1}{2}, 0$ of the *C*-centring translation to the coordinate triplets (1) to (4).

The space group has five special positions with Wyckoff letters *a* to *e*. The positions 4*a* to 4*d* require inversion symmetry, $\bar{1}$, whereas Wyckoff position 4*e* requires twofold rotation symmetry, 2, for any object in such a position. For position 4*e*, for instance, the four equivalent points have the coordinates $0, y, \frac{1}{4}$; $0, \bar{y}, \frac{3}{4}$; $\frac{1}{2}, y+\frac{1}{2}, \frac{1}{4}$; $\frac{1}{2}, \bar{y}+\frac{1}{2}, \frac{3}{4}$. The values of x and z are specified, whereas y may take any value. Since each point of position 4*e* is mapped onto itself by a twofold rotation, the multiplicity of the position is reduced from 8 to 4, whereas the order of the site-symmetry group is increased from 1 to 2.

From the symmetry-element diagram of *C*2/*c*, the locations of the four twofold axes can be deduced as $0, y, \frac{1}{4}$; $0, y, \frac{3}{4}$; $\frac{1}{2}, y, \frac{1}{4}$; $\frac{1}{2}, y, \frac{3}{4}$.

From this example, the general rule is apparent that the product of the position multiplicity and the order of the corresponding site-symmetry group is constant for all Wyckoff positions of a given space group; it is the multiplicity of the general position.

Attention is drawn to ambiguities in the description of crystal structures in a few space groups, depending on whether the coordinate triplets of *IT* (1952) or of this edition are taken. This problem is analysed by Parthé *et al.* (1988).

[2] The term *Position* (singular) is defined as a *set* of symmetry-equivalent points, in agreement with *IT* (1935): Point position; *Punktlage* (German); *position* (French). Note that in *IT* (1952) the plural, equivalent positions, was used.

2.1.3.12. Oriented site-symmetry symbols

The third column of each Wyckoff position gives the *Site symmetry*[3] of that position. The site-symmetry group is isomorphic to a (proper or improper) subgroup of the point group to which the space group under consideration belongs. The site-symmetry groups of the different points of the same special position are conjugate (symmetry-equivalent) subgroups of the space group. For this reason, all points of one special position are described by the same site-symmetry symbol. (See Section 1.4.4 for a detailed discussion of site-symmetry groups.)

Oriented site-symmetry symbols (*cf.* Fischer *et al.*, 1973) are employed to show how the symmetry elements at a site are related to the symmetry elements of the crystal lattice. The site-symmetry symbols display the same sequence of symmetry directions as the space-group symbol (*cf.* Table 2.1.3.1). Sets of equivalent symmetry directions that do not contribute any element to the site-symmetry group are represented by a dot. In this way, the orientation of the symmetry elements at the site is emphasized, as illustrated by the following examples.

Examples

(1) In the tetragonal space group $P4_22_12$ (94), Wyckoff position 4*f* has site symmetry ..2 and position 2*b* has site symmetry 2.22. The easiest way to interpret the symbols is to look at the dots first. For position 4*f*, the 2 is preceded by two dots and thus must belong to a tertiary symmetry direction. Only one tertiary direction is used. Consequently, the site symmetry is the monoclinic point group 2 with one of the two tetragonal tertiary directions as twofold axis.
Position *b* has one dot, with one symmetry symbol before and two symmetry symbols after it. The dot corresponds, therefore, to the secondary symmetry directions. The first symbol 2 indicates a twofold axis along the primary symmetry direction (*c* axis). The final symbols 22 indicate two twofold axes along the two mutually perpendicular tertiary directions $[1\bar{1}0]$ and [110]. The site symmetry is thus orthorhombic, 222.

(2) In the cubic space group *I*23 (197), position 6*b* has 222.. as its oriented site-symmetry symbol. The orthorhombic group 222 is completely related to the primary set of cubic symmetry directions, with the three twofold axes parallel to the three equivalent primary directions [100], [010], [001].

(3) In the cubic space group $Pn\bar{3}n$ (222), position 6*b* has 42.2 as its site-symmetry symbol. This 'cubic' site-symmetry symbol displays a tetragonal site symmetry. The position of the dot indicates that there is no symmetry along the four secondary cubic directions. The fourfold axis is connected with one of the three primary cubic symmetry directions and two equivalent twofold axes occur along the remaining two primary directions. Moreover, the group contains two mutually perpendicular (equivalent) twofold axes along those two of the six tertiary cubic directions ⟨110⟩ that are normal to the fourfold axis. Each pair of equivalent twofold axes is given by just one symbol 2. (Note that at the six sites of position 6*b* the fourfold axes are twice oriented along *a*, twice along *b* and twice along *c*.)

(4) In the tetragonal space group $P4_2/nnm$ (134), position 2*a* has site symmetry $\bar{4}2m$. The site has symmetry for all symmetry directions. Because of the presence of the primary $\bar{4}$ axis, only one of the twofold axes along the two secondary directions need be given explicitly and similarly for the mirror planes *m* perpendicular to the two tertiary directions.

The above examples show:

(i) The oriented site-symmetry symbols become identical to Hermann–Mauguin point-group symbols if the dots are omitted.

(ii) Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system than the space group under consideration.

To show, for the same type of site symmetry, how the oriented site-symmetry symbol depends on the space group under discussion, the site-symmetry group *mm*2 will be considered in orthorhombic and tetragonal space groups. Relevant crystal classes are *mm*2, *mmm*, 4*mm*, $\bar{4}2m$ and $4/mmm$. The site symmetry *mm*2 contains two mutually perpendicular mirror planes intersecting in a twofold axis.

For space groups of crystal class *mm*2, the twofold axis at the site must be parallel to the one direction of the rotation axes of the space group. The site-symmetry group *mm*2, therefore, occurs only in the orientation *mm*2. For space groups of class *mmm* (full symbol $2/m\ 2/m\ 2/m$), the twofold axis at the site may be parallel to *a*, *b* or *c* and the possible orientations of the site symmetry are 2*mm*, *m*2*m* and *mm*2. For space groups of the tetragonal crystal class 4*mm*, the twofold axis of the site-symmetry group *mm*2 must be parallel to the fourfold axis of the crystal. The two mirror planes must belong either to the two secondary or to the two tertiary tetragonal directions so that 2*mm*. and 2.*mm* are possible site-symmetry symbols. Similar considerations apply to class $\bar{4}2m$, which can occur in two settings, $\bar{4}2m$ and $\bar{4}m2$. Finally, for class $4/mmm$ (full symbol $4/m\ 2/m\ 2/m$), the twofold axis of 2*mm* may belong to any of the three kinds of symmetry directions and possible oriented site symmetries are 2*mm*., 2.*mm*, *m*2*m*. and *m*.2*m*. In the first two symbols, the twofold axis extends along the single primary direction and the mirror planes occupy either both secondary or both tertiary directions; in the last two cases, one mirror plane belongs to the primary direction and the second to either one secondary or one tertiary direction (the other equivalent direction in each case being occupied by the twofold axis).

2.1.3.13. Reflection conditions

The *Reflection conditions*[4] are listed in the right-hand column of each Wyckoff position.

These conditions are formulated here, in accordance with general practice, as 'conditions of occurrence' (structure factor not systematically zero) and not as 'extinctions' or 'systematic absences' (structure factor zero). Reflection conditions are listed for *all* those three-, two- and one-dimensional sets of reflections for which extinctions exist; hence, for those nets or rows that are *not* listed, no reflection conditions apply. The theoretical background of reflection conditions and their derivation are discussed in detail in Section 1.6.3.

[3] Often called point symmetry: *Punktsymmetrie* or *Lagesymmetrie* (German): *symétrie ponctuelle* (French).

[4] The reflection conditions were called *Auslöschungen* (German), missing spectra (English) and *extinctions* (French) in *IT* (1935) and 'Conditions limiting possible reflections' in *IT* (1952); they are often referred to as 'Systematic or space-group absences' (*cf.* Section 3.3.3).

There are two types of systematic reflection conditions for diffraction of radiation by crystals:

(1) *General conditions*. They are associated with systematic absences caused by the presence of lattice centrings, screw axes and glide planes. The general conditions are always obeyed, irrespective of which Wyckoff positions are occupied by atoms in a particular crystal structure.
(2) *Special conditions* ('extra' conditions). They apply only to *special* Wyckoff positions and always occur in addition to the general conditions of the space group. Note that each extra condition is valid only for the scattering contribution of those atoms that are located in the relevant special Wyckoff position. If the special position is occupied by atoms whose scattering power is high in comparison with the other atoms in the structure, reflections violating the extra condition will be weak. One should note that the special conditions apply only to isotropic and spherical atoms (*cf.* Section 1.6.3).

General reflection conditions. These are due to one of three effects:

(i) *Centred cells*. The resulting conditions apply to the whole three-dimensional set of reflections *hkl*. Accordingly, they are called *integral reflection conditions*. They are given in Table 2.1.3.6. These conditions result from the centring vectors of centred cells. They disappear if a primitive cell is chosen instead of a centred cell. Note that the centring symbol and the corresponding integral reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $C \rightarrow A \rightarrow I$).
(ii) *Glide planes*. The resulting conditions apply only to two-dimensional sets of reflections, *i.e.* to reciprocal-lattice nets containing the origin (such as *hk*0, *h*0*l*, 0*kl, hhl*). For this reason, they are called *zonal reflection conditions*. The indices *hkl* of these 'zonal reflections' obey the relation $hu + kv + lw = 0$, where $[uvw]$, the direction of the zone axis, is normal to the reciprocal-lattice net. Note that the symbol of a glide plane and the corresponding zonal reflection condition may change with a change of the basis vectors (*e.g.* monoclinic: $c \rightarrow n \rightarrow a$).
(iii) *Screw axes*. The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows containing the origin (such as *h*00, 0*k*0, 00*l*). They are called *serial reflection conditions*. It is interesting to note that some diagonal screw axes do not give rise to systematic absences (*cf.* Section 1.6.3 for more details).

Reflection conditions of types (ii) and (iii) are listed in Table 2.1.3.7. They can be understood as follows: Zonal and serial reflections form two- or one-dimensional sections through the origin of reciprocal space. In direct space, they correspond to projections of a crystal structure onto a plane or onto a line. Glide planes or screw axes may reduce the translation periods in these projections (*cf.* Section 2.1.3.14) and thus decrease the size of the projected cell. As a consequence, the cells in the corresponding reciprocal-lattice sections are increased, which means that systematic absences of reflections occur.

For the two-dimensional groups, the reasoning is analogous. The reflection conditions for the plane groups are assembled in Table 2.1.3.8.

For the *interpretation of observed reflections*, the general reflection conditions must be studied in the order (i) to (iii), as conditions of type (ii) may be included in those of type (i), while conditions of type (iii) may be included in those of types (i) or (ii). This is shown in the example below.

Table 2.1.3.6
Integral reflection conditions for centred cells (lattices)

Reflection condition	Centring type of cell	Centring symbol
None	Primitive	P
		R† (rhombohedral axes)
$h + k = 2n$	C-face centred	C
$k + l = 2n$	A-face centred	A
$h + l = 2n$	B-face centred	B
$h + k + l = 2n$	Body centred	I
$h + k$, $h + l$ and $k + l = 2n$ or: h, k, l all odd or all even ('unmixed')	All-face centred	F
$-h + k + l = 3n$	Rhombohedrally centred, obverse setting (standard)	R† (hexagonal axes)
$h - k + l = 3n$	Rhombohedrally centred, reverse setting	R† (hexagonal axes)
$h - k = 3n$	Hexagonally centred	H‡

† For further explanations see Section 2.1.1 and Table 2.1.1.2.
‡ For the use of the unconventional H cell, see Section 1.5.4 and Table 2.1.1.2.

In the *space-group tables*, the reflection conditions are given according to the following rules:

(i) for a given space group, all reflection conditions [up to symmetry equivalence, *cf.* rule (v)] are listed; hence for those nets or rows that are *not* listed no conditions apply. No distinction is made between 'independent' and 'included' conditions, as was done in *IT* (1952), where 'included' conditions were placed in parentheses;
(ii) the integral condition, if present, is always listed first, followed by the zonal and serial conditions;
(iii) conditions that have to be satisfied simultaneously are separated by a comma or by 'AND'. Thus, if two indices must be even, say h and l, the condition is written $h, l = 2n$ rather than $h = 2n$ and $l = 2n$. The same applies to sums of indices. Thus, there are several different ways to express the integral conditions for an F-centred lattice: '$h + k, h + l, k + l = 2n$' or '$h + k, h + l = 2n$ and $k + l = 2n$' or '$h + k = 2n$ and $h + l, k + l = 2n$' (*cf.* Table 2.1.3.6);
(iv) conditions separated by 'OR' are alternative conditions. For example, '*hkl*: $h = 2n + 1$ or $h + k + l = 4n$' means that *hkl* is 'present' if either the condition $h = 2n + 1$ *or* the alternative condition $h + k + l = 4n$ is fulfilled. Obviously, *hkl* is also a 'present' reflection if both conditions are satisfied. Note that 'or' conditions occur only for the *special conditions* described below;
(v) in crystal systems with two or more symmetry-equivalent nets or rows (tetragonal and higher), only *one* representative set (the first one in Table 2.1.3.7) is listed; *e.g.* tetragonal: only the first members of the equivalent sets 0*kl* and *h*0*l* or *h*00 and 0*k*0 are listed;
(vi) for cubic space groups, it is stated that the indices *hkl* are 'cyclically permutable' or 'permutable'. The cyclic permutability of h, k and l in all rhombohedral space groups, described with 'rhombohedral axes', and of h and k in some tetragonal space groups are not stated;

Table 2.1.3.7
Zonal and serial reflection conditions for glide planes and screw axes (*cf.* Table 2.1.2.1)

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane: Orientation of plane	Glide plane: Glide vector	Glide plane: Symbol	Crystallographic coordinate system to which condition applies	
$0kl$	$k = 2n$	(100)	$\mathbf{b}/2$	b	Monoclinic (a unique), Tetragonal	Orthorhombic, Cubic
	$l = 2n$		$\mathbf{c}/2$	c		
	$k + l = 2n$		$\mathbf{b}/2 + \mathbf{c}/2$	n		
	$k + l = 4n$ $(k, l = 2n)$ †		$\mathbf{b}/4 \pm \mathbf{c}/4$	d		
$h0l$	$l = 2n$	(010)	$\mathbf{c}/2$	c	Monoclinic (b unique), Tetragonal	Orthorhombic, Cubic
	$h = 2n$		$\mathbf{a}/2$	a		
	$l + h = 2n$		$\mathbf{c}/2 + \mathbf{a}/2$	n		
	$l + h = 4n$ $(l, h = 2n)$ †		$\mathbf{c}/4 \pm \mathbf{a}/4$	d		
$hk0$	$h = 2n$	(001)	$\mathbf{a}/2$	a	Monoclinic (c unique), Tetragonal	Orthorhombic, Cubic
	$k = 2n$		$\mathbf{b}/2$	b		
	$h + k = 2n$		$\mathbf{a}/2 + \mathbf{b}/2$	n		
	$h + k = 4n$ $(h, k = 2n)$ †		$\mathbf{a}/4 \pm \mathbf{b}/4$	d		
$h\bar{h}0l$ $0k\bar{k}l$ $\bar{h}0hl$	$l = 2n$	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ } $\{11\bar{2}0\}$	$\mathbf{c}/2$	c	Hexagonal	
$hh.\overline{2h}.l$ $\overline{2h}.hhl$ $h.\overline{2h}.hl$	$l = 2n$	$(1\bar{1}00)$ $(01\bar{1}0)$ $(\bar{1}010)$ } $\{1\bar{1}00\}$	$\mathbf{c}/2$	c	Hexagonal	
hhl	$l = 2n$	$(1\bar{1}0)$ } $\{1\bar{1}0\}$	$\mathbf{c}/2$	c, n	Rhombohedral‡	
hkk	$h = 2n$	$(01\bar{1})$	$\mathbf{a}/2$	a, n		
hkh	$k = 2n$	$(\bar{1}01)$	$\mathbf{b}/2$	b, n		
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0), (110)$	$\mathbf{c}/2$	c, n	Tetragonal§	Cubic¶
	$2h + l = 4n$		$\mathbf{a}/4 \pm \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkk, hk\bar{k}$	$h = 2n$	$(01\bar{1}), (011)$	$\mathbf{a}/2$	a, n		
	$2k + h = 4n$		$\pm\mathbf{a}/4 + \mathbf{b}/4 \pm \mathbf{c}/4$	d		
$hkh, \bar{h}kh$	$k = 2n$	$(\bar{1}01), (101)$	$\mathbf{b}/2$	b, n		
	$2h + k = 4n$		$\pm\mathbf{a}/4 \pm \mathbf{b}/4 + \mathbf{c}/4$	d		

† Glide planes *d* with orientations (100), (010) and (001) occur only in orthorhombic and cubic *F* space groups. Combination of the integral reflection condition (*hkl:* all odd or all even) with the zonal conditions for the *d* glide planes leads to the further conditions given between parentheses.
‡ For rhombohedral space groups described with 'rhombohedral axes', the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, and *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, *c* is always used, as in $R3c$ (161) and $R\bar{3}c$ (167), because *c* glides also occur in the hexagonal description of these space groups.
§ For tetragonal *P* space groups, the two reflection conditions (*hhl* and $h\bar{h}l$ with $l = 2n$) imply interleaving of *c* and *n* glides. In the Hermann–Mauguin space-group symbols, *c* is always used, irrespective of which glide planes contain the origin: *cf.* $P4cc$ (103), $P\bar{4}2c$ (112) and $P4/nnc$ (126).
¶ For cubic space groups, the three reflection conditions ($l = 2n, h = 2n, k = 2n$) imply interleaving of *c* and *n* glides, *a* and *n* glides, and *b* and *n* glides, respectively. In the Hermann–Mauguin space-group symbols, either *c* or *n* is used, depending upon which glide plane contains the origin, *cf.* $P\bar{4}3n$ (218), $Pn\bar{3}n$ (222), $Pm\bar{3}n$ (223) *versus* $F\bar{4}3c$ (219), $Fm\bar{3}c$ (226), $Fd\bar{3}c$ (228).

(vii) in the 'hexagonal-axes' descriptions of trigonal and hexagonal space groups, Bravais–Miller indices *hkil* are used. They obey two conditions:

(*a*) $h + k + i = 0$, *i.e.* $i = -(h + k)$;
(*b*) the indices h, k, i are cyclically permutable; this is not stated. Further details can be found in textbooks of crystallography.

Note that the integral reflection conditions for a rhombohedral lattice, described with 'hexagonal axes', permit the presence of only one member of the pair *hkil* and $\bar{h}\bar{k}\bar{i}l$ for $l \neq 3n$ (*cf.* Table 2.1.3.6). This applies also to the zonal reflections $h\bar{h}0l$ and $\bar{h}h0l$, which for the rhombohedral space groups must be considered separately.

Example

For a monoclinic crystal (*b* unique), the following reflection conditions have been observed:

(1) hkl: $h + k = 2n$;
(2) $0kl$: $k = 2n$; $h0l$: $h, l = 2n$; $hk0$: $h + k = 2n$;
(3) $h00$: $h = 2n$; $0k0$: $k = 2n$; $00l$: $l = 2n$.

Line (1) states that the cell used for the description of the space group is *C* centred. In line (2), the conditions $0kl$ with $k = 2n$, $h0l$ with $h = 2n$ and $hk0$ with $h + k = 2n$ are a consequence of the integral condition (1), leaving only $h0l$ with $l = 2n$ as a new condition. This indicates a glide plane *c*. Line (3) presents no new condition, since $h00$ with $h = 2n$ and $0k0$ with $k = 2n$ follow from the integral condition (1), whereas $00l$

Table 2.1.3.7 (continued)

(*b*) Screw axes

Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies
		Direction of axis	Screw vector	Symbol	
*h*00	$h = 2n$	[100]	**a**/2	2_1	Monoclinic (*a* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$h = 4n$		**a**/4	$4_1, 4_3$	
0*k*0	$k = 2n$	[010]	**b**/2	2_1	Monoclinic (*b* unique), Orthorhombic, Tetragonal; Cubic
				4_2	
	$k = 4n$		**b**/4	$4_1, 4_3$	
00*l*	$l = 2n$	[001]	**c**/2	2_1	Monoclinic (*c* unique), Orthorhombic; Tetragonal; Cubic
				4_2	
	$l = 4n$		**c**/4	$4_1, 4_3$	
000*l*	$l = 2n$	[001]	**c**/2	6_3	Hexagonal
	$l = 3n$		**c**/3	$3_1, 3_2, 6_2, 6_4$	
	$l = 6n$		**c**/6	$6_1, 6_5$	

with $l = 2n$ is a consequence of a zonal condition (2). Accordingly, there need not be a twofold screw axis along [010]. Space groups obeying the conditions are *Cc* (9, *b* unique, cell choice 1) and *C*2/*c* (15, *b* unique, cell choice 1). Under certain conditions, using methods based on resonant scattering, it is possible to determine whether the structure space group is centrosymmetric or not (*cf.* Section 1.6.5.1).

For a different choice of the basis vectors, the reflection conditions would appear in a different form owing to the transformation of the reflection indices (*cf.* cell choices 2 and 3 for space groups *Cc* and *C*2/*c* in Chapter 2.3). The transformations of reflection conditions under coordinate transformations are discussed and illustrated in Sections 1.5.2 and 1.5.3.

Special or 'extra' reflection conditions. These apply either to the integral reflections *hkl* or to particular sets of zonal or serial reflections. In the space-group tables, the minimal special conditions are listed that, on combination with the general conditions, are sufficient to generate the complete set of conditions. This will be apparent from the examples below.

Examples

(1) $P4_222$ (93)

General position 8*p*: 00*l*: $l = 2n$, due to 4_2; the projection on [001] of any crystal structure with this space group has periodicity $\frac{1}{2}c$.

Special position 4*i*: *hkl*: $h + k + l = 2n$; any set of symmetry-equivalent atoms in this position displays additional *I* centring.

Special position 4*n*: 0*kl*: $l = 2n$; any set of equivalent atoms in this position displays a glide plane $c \perp [100]$. Projection of this set along [100] results in a halving of the original *c* axis, hence the special condition. Analogously for *h*0*l*: $l = 2n$.

(2) *C*12/*c*1 (15, unique axis *b*, cell choice 1)

General position 8*f*: *hkl*: $h + k = 2n$, due to the *C*-centred cell.

Special position 4*d*: *hkl*: $k + l = 2n$, due to additional *A* and *B* centring for atoms in this position. Combination with the general condition results in *hkl*: $h + k, h + l$, $k + l = 2n$ or *hkl* all odd or all even; this corresponds to an *F*-centred arrangement of atoms in this position.

Special position 4*b*: *hkl*: $l = 2n$, due to additional halving of the *c* axis for atoms in this position. Combination with the general condition results in *hkl*: $h + k, l = 2n$; this corresponds to a *C*-centred arrangement in a cell with half the original *c* axis. No further condition results from the combination.

(3) *I*12/*a*1 (15, unique axis *b*, cell choice 3)

For the description of space group No. 15 with cell choice 3 (see Section 2.1.3.15 and the space-group tables), the reflection conditions appear as follows:

General position 8*f*: *hkl*: $h + k + l = 2n$, due to the *I*-centred cell.

Special position 4*b*: *hkl*: $h = 2n$, due to additional halving of the *a* axis. Combination gives *hkl*: $h, k + l = 2n$, *i.e.* an *A*-centred arrangement of atoms in a cell with half the original *a* axis.

An analogous result is obtained for position 4*d*.

Table 2.1.3.8
Reflection conditions for the plane groups

Type of reflections	Reflection condition	Centring type of plane cell; or glide line with glide vector	Coordinate system to which condition applies
hk	None	Primitive *p*	All systems
	$h + k = 2n$	Centred *c*	Rectangular
	$h - k = 3n$	Hexagonally centred *h*†	Hexagonal
*h*0	$h = 2n$	Glide line *g* normal to *b* axis; glide vector $\frac{1}{2}\mathbf{a}$	Rectangular, Square
0*k*	$k = 2n$	Glide line *g* normal to *a* axis; glide vector $\frac{1}{2}\mathbf{b}$	

† For the use of the unconventional *h* cell see Table 2.1.1.2.

(4) *Fmm*2 (42)

General position 16*e*: *hkl*: $h + k, h + l, k + l = 2n$, due to the *F*-centred cell.

Special position 8*b*: *hkl*: $= 2n$, due to additional halving of the *a* axis. Combination results in *hkl*: $h, k, l = 2n$, *i.e.* all indices even; the atoms in this position are arranged in a primitive lattice with axes $\frac{1}{2}a$, $\frac{1}{2}b$ and $\frac{1}{2}c$.

For the cases where the special reflection conditions are described by means of combinations of 'OR' and 'AND' instructions, the 'AND' condition always has to be evaluated with priority, as shown by the following example.

Example: P$\bar{4}$3*n (218)*

Special position 6*d*: *hkl*: $h + k + l = 2n$ or $h = 2n + 1, k = 4n$ and $l = 4n + 2$.

This expression contains the following two conditions:

(*a*) *hkl*: $h + k + l = 2n$;

(*b*) $h = 2n + 1$ and $k = 4n$ and $l = 4n + 2$.

A reflection is 'present' (occurring) if either condition (*a*) is satisfied or if a permutation of the three conditions in (*b*) are simultaneously fulfilled.

Structural or non-space-group absences. Note that in addition *non-space-group absences* may occur that are not due to the symmetry of the space group (*i.e.* centred cells, glide planes or screw axes). Atoms in general or special positions may cause additional systematic absences if their coordinates assume special values [*e.g.* 'noncharacteristic orbits'; *cf.* Section 1.4.4.4 and Engel *et al.* (1984)]. Non-space-group absences may also occur for special arrangements of atoms ('false symmetry') in a crystal structure (*cf.* Templeton, 1956; Sadanaga *et al.*, 1978). Non-space-group absences may occur also for polytypic structures; this is briefly discussed by Durovič in Section 9.2.2.2.5 of *International Tables for Crystallography* (2004), Vol. C. Even though all these 'structural absences' are fortuitous and due to the special arrangements of atoms in a particular crystal structure, they have the appearance of space-group absences. Occurrence of structural absences thus may lead to an *incorrect assignment of the space group*. Accordingly, the reflection conditions in the space-group tables must be considered as a minimal set of conditions.

The use of reflection conditions and of the symmetry of reflection intensities for space-group determination is described in Chapter 1.6.

2.1.3.14. Symmetry of special projections

Projections of crystal structures are used by crystallographers in special cases. Use of so-called 'two-dimensional data' (zero-layer intensities) results in the projection of a crystal structure along the normal to the reciprocal-lattice net. A detailed treatment of projections of space groups, including basic definitions and illustrative examples, is given in Section 1.4.5.3.

Even though the projection of a finite object along *any* direction may be useful, the projection of a *periodic* object such as a crystal structure is only sensible along a rational lattice direction (lattice row). Projection along a nonrational direction results in a constant density in at least one direction.

Data listed in the space-group tables. Under the heading *Symmetry of special projections*, the following data are listed for three projections of each space group; no projection data are given for the plane groups.

(i) *The projection direction*. All projections are orthogonal, *i.e.* the projection is made onto a plane normal to the projection direction. This ensures that spherical atoms appear as circles in the projection. For each space group, three projections are listed. If a lattice has three kinds of symmetry directions, the three projection directions correspond to the primary, secondary and tertiary symmetry directions of the lattice (*cf.* Table 2.1.3.1). If a lattice contains fewer than three kinds of symmetry directions, as in the triclinic, monoclinic and rhombohedral cases, the additional projection direction(s) are taken along coordinate axes, *i.e.* lattice rows lacking symmetry.

The directions for which projection data are listed are as follows:

Triclinic Monoclinic (both settings) Orthorhombic	[001]	[100]	[010]
Tetragonal	[001]	[100]	[110]
Hexagonal	[001]	[100]	[210]
Rhombohedral	[111]	[1$\bar{1}$0]	[2$\bar{1}\bar{1}$]
Cubic	[001]	[111]	[110]

(ii) *The Hermann–Mauguin symbol of the plane group* resulting from the projection of the space group. If necessary, the symbols are given in oriented form; for example, plane group *pm* is expressed either as *p*1*m*1 or as *p*11*m* (*cf.* Section 1.4.1.5 for explanations of Hermann–Mauguin symbols of plane groups).

(iii) *Relations between the basis vectors* $\mathbf{a}'$, $\mathbf{b}'$ of the plane group and the basis vectors **a**, **b**, **c** of the space group. Each set of basis vectors refers to the conventional coordinate system of the plane group or space group, as employed in Chapters 2.2 and 2.3. The basis vectors of the two-dimensional cell are always called $\mathbf{a}'$ and $\mathbf{b}'$ irrespective of which two of the basis vectors **a**, **b**, **c** of the three-dimensional cell are projected to form the plane cell. All relations between the basis vectors of the two cells are expressed as vector equations, *i.e.* $\mathbf{a}'$ and $\mathbf{b}'$ are given as linear combinations of **a**, **b** and **c**. For the triclinic or monoclinic space groups, basis vectors **a**, **b** or **c** inclined to the plane of projection are replaced by the projected vectors $\mathbf{a}_p$, $\mathbf{b}_p$, $\mathbf{c}_p$.

For primitive three-dimensional cells, the *metrical* relations between the lattice parameters of the space group and the plane group are collected in Table 2.1.3.9. The additional relations for centred cells can be derived easily from the table.

(iv) *Location of the origin* of the plane group with respect to the unit cell of the space group. The same description is used as for the location of symmetry elements (*cf.* Section 2.1.3.9).

Example

'Origin at *x*, 0, 0' or 'Origin at $\frac{1}{4}, \frac{1}{4}, z$'.

Projections of centred cells (lattices). For centred lattices, two different cases may occur:

(i) The projection direction is parallel to a lattice-centring vector. In this case, the projected plane cell is primitive for the centring types *A*, *B*, *C*, *I* and *R*. For *F*-centred lattices, the multiplicity is reduced from 4 to 2 because *c*-centred plane

Table 2.1.3.9
Cell parameters a', b', γ' of the two-dimensional cell in terms of cell parameters a, b, c, α, β, γ of the three-dimensional cell for the projections listed in the space-group tables of Chapter 2.3

Projection direction	Triclinic	Monoclinic		Orthorhombic
		Unique axis b	Unique axis c	
[001]	$a' = a \sin\beta$ $b' = b \sin\alpha$ $\gamma' = 180^\circ - \gamma^*$†	$a' = a \sin\beta$ $b' = b$ $\gamma' = 90^\circ$	$a' = a$ $b' = b$ $\gamma' = \gamma$	$a' = a$ $b' = b$ $\gamma' = 90^\circ$
[100]	$a' = b \sin\gamma$ $b' = c \sin\beta$ $\gamma' = 180^\circ - \alpha^*$†	$a' = b$ $b' = c \sin\beta$ $\gamma' = 90^\circ$	$a' = b \sin\gamma$ $b' = c$ $\gamma' = 90^\circ$	$a' = b$ $b' = c$ $\gamma' = 90^\circ$
[010]	$a' = c \sin\alpha$ $b' = \alpha \sin\gamma$ $\gamma' = 180^\circ - \beta^*$†	$a' = c$ $b' = a$ $\gamma' = \beta$	$a' = c$ $b' = a \sin\gamma$ $\gamma' = 90^\circ$	$a' = c$ $b' = a$ $\gamma' = 90^\circ$

Projection direction	Tetragonal
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$
[100]	$a' = a$ $b' = c$ $\gamma' = 90^\circ$
[110]	$a' = (a/2)\sqrt{2}$ $b' = c$ $\gamma' = 90^\circ$

Projection direction	Hexagonal
[001]	$a' = a$ $b' = a$ $\gamma' = 120^\circ$
[100]	$a' = (a/2)\sqrt{3}$ $b' = c$ $\gamma' = 90^\circ$
[210]	$a' = a/2$ $b' = c$ $\gamma' = 90^\circ$

Projection direction	Rhombohedral‡
[111]	$a' = \frac{2}{\sqrt{3}} a \sin(\alpha/2)$ $b' = \frac{2}{\sqrt{3}} a \sin(\alpha/2)$ $\gamma' = 120^\circ$
$[1\bar{1}0]$	$a' = a \cos(\alpha/2)$ $b' = a$ $\gamma' = \delta$§
$[\bar{2}11]$	$a' = \frac{1}{\sqrt{3}} a\sqrt{1 + 2\cos\alpha}$ $b' = a \sin(\alpha/2)$ $\gamma' = 90^\circ$

Projection direction	Cubic
[001]	$a' = a$ $b' = a$ $\gamma' = 90^\circ$
[111]	$a' = a\sqrt{2/3}$ $b' = a\sqrt{2/3}$ $\gamma' = 120^\circ$
[110]	$a' = (a/2)\sqrt{2}$ $b' = a$ $\gamma' = 90^\circ$

† $\cos\alpha^* = \dfrac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$; $\cos\beta^* = \dfrac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha}$; $\cos\gamma^* = \dfrac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$.

‡ The entry 'Rhombohedral' refers to the primitive rhombohedral cell with $a = b = c$, $\alpha = \beta = \gamma$ (*cf.* Table 2.1.1.1).

§ $\cos\delta = \dfrac{\cos\alpha}{\cos\alpha/2}$.

cells result from projections along face diagonals of three-dimensional F cells.

Examples

(1) A body-centred lattice with centring vector $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$ gives a primitive net if projected along [111], $[\bar{1}11]$, $[1\bar{1}1]$ or $[11\bar{1}]$.
(2) A C-centred lattice projects to a primitive net along the directions [110] and $[1\bar{1}0]$.
(3) An R-centred lattice described with 'hexagonal axes' (triple cell) results in a primitive net if projected along $[\bar{1}11]$, [211] or $[\bar{1}\bar{2}1]$ for the obverse setting. For the reverse setting, the corresponding directions are $[1\bar{1}1]$, $[\bar{2}\bar{1}1]$, [121]; *cf.* Table 2.1.1.2.

(ii) The projection direction is not parallel to a lattice-centring vector (general projection direction). In this case, the plane cell has the same multiplicity as the three-dimensional cell. Usually, however, this centred plane cell is unconventional and a transformation is required to obtain the conventional plane cell. This transformation has been carried out for the projection data in this volume.

Examples

(1) Projection along [010] of a cubic I-centred cell leads to an unconventional quadratic c-centred plane cell. A simple cell transformation leads to the conventional quadratic p cell.
(2) Projection along [010] of an orthorhombic I-centred cell leads to a rectangular c-centred plane cell, which is conventional.
(3) Projection along [001] of an R-centred cell (both in obverse and reverse setting) results in a triple hexagonal plane cell h (the two-dimensional analogue of the H cell, *cf.* Table 2.1.1.2). A simple cell transformation leads to the conventional hexagonal p cell.

Table 2.1.3.10
Projections of crystallographic symmetry elements

Symmetry element in three dimensions	Symmetry element in projection
Arbitrary orientation	
Symmetry centre $\bar{1}$ Rotoinversion axis $\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Parallel to projection direction	
Rotation axis 2; 3; 4; 6	Rotation point 2; 3; 4; 6
Screw axis 2_1	Rotation point 2
$3_1, 3_2$	3
$4_1, 4_2, 4_3$	4
$6_1, 6_2, 6_3, 6_4, 6_5$	6
Rotoinversion axis $\bar{4}$	Rotation point 4
$\bar{6} \equiv 3/m$	3, with overlap of atoms
$\bar{3} \equiv 3 \times \bar{1}$	6
Reflection plane *m*	Reflection line *m*
Glide plane with ⊥ component†	Glide line *g*
Glide plane without ⊥ component†	Reflection line *m*
Normal to projection direction	
Rotation axis 2;4;6	Reflection line *m*
3	None
Screw axis 4_2; $6_2, 6_4$	Reflection line *m*
2_1; $4_1, 4_3$; $6_1, 6_3, 6_5$	Glide line *g*
$3_1, 3_2$	None
Rotoinversion axis $\bar{4}$	Reflection line *m* parallel to axis
$\bar{6} \equiv 3/m$	Reflection line *m* perpendicular to axis (through projection of inversion point)
$\bar{3} \equiv 3 \times \bar{1}$	Rotation point 2 (at projection of centre)
Reflection plane *m*	None, but overlap of atoms
Glide plane with glide vector **t**	Translation with translation vector **t**

† The term 'with ⊥ component' refers to the component of the glide vector normal to the projection direction.

Projections of symmetry elements. A symmetry element of a space group does not project as a symmetry element unless its orientation bears a special relation to the projection direction; all translation components of a symmetry operation along the projection direction vanish, whereas those perpendicular to the projection direction (*i.e.* parallel to the plane of projection) may be retained. This is summarized in Table 2.1.3.10 for the various crystallographic symmetry elements. From this table the following conclusions can be drawn:

(i) *n*-fold rotation axes and *n*-fold screw axes, as well as rotoinversion axes $\bar{4}$, *parallel to the projection direction* project as *n*-fold rotation points; a $\bar{3}$ axis projects as a sixfold, a $\bar{6}$ axis as a threefold rotation point. For the latter, a doubling of the projected electron density occurs owing to the mirror plane normal to the projection direction ($\bar{6} \equiv 3/m$).

(ii) *n*-fold rotation axes and *n*-fold screw axes *normal to the projection direction* (*i.e.* parallel to the plane of projection) do not project as symmetry elements if *n* is odd. If *n* is even, all rotation and rotoinversion axes project as mirror lines: the same applies to the screw axes 4_2, 6_2 and 6_4 because they contain an axis 2. Screw axes 2_1, 4_1, 4_3, 6_1, 6_3 and 6_5 project as glide lines because they contain 2_1.

(iii) Reflection planes *normal* to the projection direction do not project as symmetry elements but lead to a doubling of the projected electron density owing to overlap of atoms. Projection of a glide plane results in an additional translation; the new translation vector is equal to the glide vector of the glide plane. Thus, a reduction of the translation period in that particular direction takes place.

(iv) Reflection planes *parallel* to the projection direction project as reflection lines. Glide planes project as glide lines or as reflection lines, depending upon whether the glide vector has or does not have a component parallel to the projection plane.

(v) Centres of symmetry, as well as $\bar{3}$ axes in *arbitrary* orientation, project as twofold rotation points.

A detailed discussion of the correspondence between the symmetry elements and their projections is given in Section 1.4.5.3.

*Example: C*12/*c*1 *(15, b unique, cell choice 1)*

The *C*-centred cell has lattice points at 0, 0, 0 and $\frac{1}{2}, \frac{1}{2}, 0$. In all projections, the centre $\bar{1}$ projects as a twofold rotation point.

Projection along [001]: The plane cell is centred; 2 ∥ [010] projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* vanishes and thus *c* projects as *m*.

Result: Plane group *c*2*mm* (9), $\mathbf{a}' = \mathbf{a}_p$, $\mathbf{b}' = \mathbf{b}$.

Projection along [100]: The periodicity along *b* is halved because of the *C* centring; 2 ∥ [010] projects as *m*; the glide component $(0, 0, \frac{1}{2})$ of glide plane *c* is retained and thus *c* projects as *g*.

Result: Plane group *p*2*gm* (7), $\mathbf{a}' = \mathbf{b}/2$, $\mathbf{b}' = \mathbf{c}_p$.

Projection along [010]: The periodicity along *a* is halved because of the *C* centring; that along *c* is halved owing to the glide component $(0, 0, \frac{1}{2})$ of glide plane *c*; 2 ∥ [010] projects as 2.

Result: Plane group *p*2 (2), $\mathbf{a}' = \mathbf{c}/2$, $\mathbf{b}' = \mathbf{a}/2$.

Further details about the geometry of projections can be found in publications by Buerger (1965) and Biedl (1966).

2.1.3.15. Monoclinic space groups

In this volume, space groups are described by one (or at most two) conventional coordinate systems (*cf.* Sections 2.1.1.2 and 2.1.3.2). Eight monoclinic space groups, however, are treated more extensively. In order to provide descriptions for frequently encountered cases, they are given in six versions.

The description of a monoclinic crystal structure in this volume, including its Hermann–Mauguin space-group symbol, depends upon two choices:

(i) the unit cell chosen, here called 'cell choice';

(ii) the labelling of the edges of this cell, especially of the monoclinic symmetry direction ('unique axis'), here called 'setting'.

Cell choices. One edge of the cell, *i.e.* one crystal axis, is always chosen along the monoclinic symmetry direction. The other two edges are located in the plane perpendicular to this direction and coincide with translation vectors in this 'monoclinic plane'. It is sensible and common practice (see below) to choose these two basis vectors from the *shortest three* translation vectors in that plane. They are shown in Fig. 2.1.3.12 and labelled **e**, **f** and **g**, in order of increasing length.[5] The two shorter vectors span the 'reduced mesh' (where mesh means a two-dimensional unit cell), here **e** and **f**; for this mesh, the monoclinic angle is $\leq 120°$,

[5] These three vectors obey the 'closed-triangle' condition $\mathbf{e} + \mathbf{f} + \mathbf{g} = \mathbf{0}$; they can be considered as two-dimensional homogeneous axes.

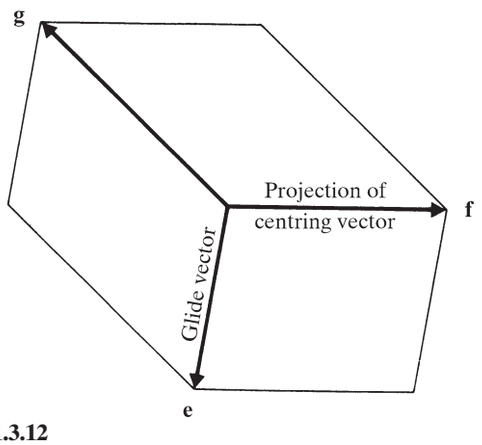


Figure 2.1.3.12
The three primitive two-dimensional cells which are spanned by the shortest three translation vectors **e**, **f**, **g** in the monoclinic plane. For the present discussion, the glide vector is considered to be along **e** and the projection of the centring vector along **f**.

whereas for the other two primitive meshes larger angles are possible.

Other choices of the basis vectors in the monoclinic plane are possible, provided they span a primitive mesh. It turns out, however, that the space-group symbol for any of these (non-reduced) meshes already occurs among the symbols for the three meshes formed by **e**, **f**, **g** in Fig. 2.1.3.12; hence only these cases need be considered. They are designated in this volume as 'cell choice 1, 2 or 3' and are depicted in Fig. 2.1.3.4. The transformation matrices for the three cell choices are listed in Table 1.5.1.1.

Settings. The term *setting* of a cell or of a space group refers to the assignment of labels (a, b, c) and directions to the edges of a given unit cell, resulting in a set of basis vectors **a**, **b**, **c**. (For orthorhombic space groups, the six settings are described and illustrated in Section 2.1.3.6.4.)

The symbol for each setting is a shorthand notation for the transformation of a given starting set **abc** into the setting considered. It is called here 'setting symbol'. For instance, the setting symbol **bca** stands for

$$\mathbf{a}' = \mathbf{b}, \quad \mathbf{b}' = \mathbf{c}, \quad \mathbf{c}' = \mathbf{a}$$

or

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = (\mathbf{b}, \mathbf{c}, \mathbf{a}),$$

where $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ is the new set of basis vectors. [Note that the setting symbol **bca** means that the 'old' vector **a** changes its label to $\mathbf{c}'$ (and not to $\mathbf{b}'$), that the 'old' vector **b** changes its label to $\mathbf{a}'$ (and not to $\mathbf{c}'$) and that the 'old' vector **c** changes its label to $\mathbf{b}'$ (and not to $\mathbf{a}'$).] Transformation of one setting into another preserves the shape of the cell and its orientation relative to the lattice. The matrices of these transformations have *one* entry +1 or −1 in each row and column; all other entries are 0.

In monoclinic space groups, one axis, the monoclinic symmetry direction, is unique. Its label must be chosen first and, depending upon this choice, one speaks of 'unique axis b', 'unique axis c' or 'unique axis a'.[6] Conventionally, the positive directions of the two further ('oblique') axes are oriented so as to make the monoclinic angle non-acute, *i.e.* $\geq 90°$, and the coordinate system right-handed. For the three cell choices, settings obeying this condition and having the same label and direction of the unique axis are considered as one setting; this is illustrated in Fig. 2.1.3.4.

Note: These three cases of labelling the monoclinic axis are often called somewhat loosely b-axis, c-axis and a-axis 'settings'. It must be realized, however, that the choice of the 'unique axis' alone does *not* define a *single* setting but only a *pair*, as for each cell the labels of the two oblique axes can be interchanged.

Table 2.1.3.11
Monoclinic setting symbols

The settings are distributed between three sets (with two columns in each set) depending on the choice of unique axis. The unique axis is underlined. The setting symbol is a shorthand notation for the transformation of the corresponding starting setting (first row **abc**; second row **abc**; third row **abc**). For example, the symbol **cab** represents a transformation of the starting setting **abc** such that $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$, $\mathbf{c}' = \mathbf{b}$.

Starting setting	Unique axis b		Unique axis c		Unique axis a	
abc	**abc**	**cba**	**cab**	**acb**	**bca**	**bac**
abc	**bca**	**acb**	**abc**	**bac**	**cab**	**cba**
abc	**cab**	**bac**	**bca**	**cba**	**abc**	**acb**

Note: An interchange of two axes involves a change of the handedness of the coordinate system. In order to keep the system right-handed, one sign reversal is necessary.

Table 2.1.3.11 lists the setting symbols for the six monoclinic settings in three equivalent forms, starting with the symbols **abc** (first line), **abc** (second line) and **abc** (third line); the unique axis is underlined. These symbols are also found in the headline of the synoptic Table 1.5.4.4, which lists the space-group symbols for all monoclinic settings and cell choices. Again, the corresponding transformation matrices are listed in Table 1.5.1.1.

In the space-group tables, only the settings with b and c unique are treated and for these only the left-hand members of the double entries in Table 2.1.3.11. This implies, for instance, that the c-axis setting is obtained from the b-axis setting by cyclic permutation of the labels, *i.e.* by the transformation

$$(\mathbf{a}', \mathbf{b}', \underline{\mathbf{c}}') = (\mathbf{a}, \underline{\mathbf{b}}, \mathbf{c}) \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = (\mathbf{c}, \mathbf{a}, \underline{\mathbf{b}}).$$

The setting with a unique is also included in the present discussion, as this setting occurs in Table 1.5.4.4. The a-axis setting $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{c}}\mathbf{ab}$ (*i.e.* $\underline{\mathbf{a}}' = \underline{\mathbf{c}}, \mathbf{b}' = \mathbf{a}, \mathbf{c}' = \mathbf{b}$) is obtained from the c-axis setting also by cyclic permutation of the labels and from the b-axis setting by the reverse cyclic permutation: $\underline{\mathbf{a}}'\mathbf{b}'\mathbf{c}' = \underline{\mathbf{b}}\mathbf{ca}$.

By the conventions described above, the setting of each of the cell choices 1, 2 and 3 is determined once the label and the direction of the unique-axis vector have been selected. Six of the nine resulting possibilities are illustrated in Fig. 2.1.3.4.

Cell choices and settings in the present tables. There are five monoclinic space groups for which the Hermann–Mauguin symbols are independent of the cell choice, *viz* those space groups that do *not* contain centred lattices or glide planes:

$$P2\ (3),\ P2_1\ (4),\ Pm\ (6),\ P2/m\ (10),\ P2_1/m\ (11).$$

In these cases, description of the space group by one cell choice is sufficient.

For the eight monoclinic space groups *with centred lattices or glide planes*, the Hermann–Mauguin symbol depends on the

[6] In *IT* (1952), the terms '1st setting' and '2nd setting' were used for 'unique axis c' and 'unique axis b'. In the present volume, as in the previous editions of this series, these terms have been dropped in favour of the latter names, which are unambiguous.

Table 2.1.3.12
Symbols for centring types and glide planes of monoclinic space groups

Setting		Cell choice		
		1	2	3
Unique axis *b*	Centring type Glide planes	*C* *c*, *n*	*A* *n*, *a*	*I* *a*, *c*
Unique axis *c*	Centring type Glide planes	*A* *a*, *n*	*B* *n*, *b*	*I* *b*, *a*
Unique axis *a*	Centring type Glide planes	*B* *b*, *n*	*C* *n*, *c*	*I* *c*, *b*

choice of the oblique axes with respect to the glide vector and/or the centring vector. These eight space groups are:

*C*2 (5), *Pc* (7), *Cm* (8), *Cc* (9), *C*2/*m* (12), *P*2/*c* (13), $P2_1/c$ (14), *C*2/*c* (15).

Here, the glide vector or the projection of the centring vector onto the monoclinic plane is always directed along *one* of the vectors **e**, **f** or **g** in Fig. 2.1.3.12, *i.e.* is parallel to the shortest, the second-shortest or the third-shortest translation vector in the monoclinic plane (note that a glide vector and the projection of a centring vector cannot be parallel). This results in three possible orientations of the glide vector or the centring vector with respect to these crystal axes, and thus in three different full Hermann–Mauguin symbols (*cf.* Section 2.1.3.4) for each setting of a space group.

Table 2.1.3.12 lists the symbols for centring types and glide planes for the cell choices 1, 2, 3. The order of the three cell choices is defined as follows: The symbols occurring in the familiar 'standard short monoclinic space-group symbols' (see Section 2.1.3.3) define cell choice 1; for 'unique axis *b*', this applies to the centring type *C* and the glide plane *c*, as in *Cm* (8) and $P2_1/c$ (14). Cell choices 2 and 3 follow from the anticlockwise order 1–2–3 in Fig. 2.1.3.4 and their space-group symbols can be obtained from Table 2.1.3.12. The *c*-axis and the *a*-axis settings then are derived from the *b*-axis setting by cyclic permutations of the axial labels, as described in this section.

In the two space groups *Cc* (9) and *C*2/*c* (15), glide planes occur in pairs, *i.e.* each vector **e**, **f**, **g** is associated either with a glide vector or with the centring vector of the cell. For *Pc* (7), *P*2/*c* (13) and $P2_1/c$ (14), which contain only one type of glide plane, the left-hand member of each pair of glide planes in Table 2.1.3.12 applies.

In the space-group tables of this volume, the following treatments of monoclinic space groups are given:

(1) *Two complete descriptions* for each of the five monoclinic space groups with primitive lattices and without glide planes, one for 'unique axis *b*' and one for 'unique axis *c*', similar to the treatment in *IT* (1952).

(2) A total of *six descriptions* for each of the eight space groups with centred lattices or glide planes, as follows:

(*a*) *One complete* description for 'unique axis *b*' and 'cell choice' 1. This is considered the standard description of the space group, and its *short* Hermann–Mauguin symbol is used as the *standard* symbol of the space group.

This standard short symbol corresponds to the one symbol of *IT* (1935) and to that of the *b*-axis setting in *IT* (1952), *e.g.* $P2_1/c$ or *C*2/*c*. It serves only to identify the space-group type but carries no information about the setting or cell choice of a particular description. The *standard short symbol* is given in the headline of every description of a monoclinic space group; *cf.* Section 2.1.3.3.

(*b*) *Three condensed* (synoptic) descriptions for 'unique axis *b*' and the three 'cell choices' 1, 2, 3. Cell choice 1 is repeated to facilitate comparison with the other cell choices. Diagrams are provided to illustrate the three cell choices: *cf.* Section 2.1.3.6.

(*c*) *One complete* description for 'unique axis *c*' and 'cell choice' 1.

(*d*) *Three condensed* (synoptic) descriptions for 'unique axis *c*' and the three 'cell choices' 1, 2, 3. Again cell choice 1 is repeated and appropriate diagrams are provided.

All settings and cell choices are identified by the appropriate *full* Hermann–Mauguin symbols (*cf.* Section 2.1.3.4), *e.g.* *C*12/*c*1 or *I*112/*b*. For the two space groups *Cc* (9) and *C*2/*c* (15) with pairs of different glide planes, the 'simplest operation rule' for reflections ($m > a$, b, $c > n$) is not followed (*cf.* Section 1.4.1). Instead, in order to bring out the relations between the various settings and cell choices, the glide-plane symbol always refers to that glide plane which intersects the conventional origin.

*Example: No. 15, standard short symbol C*2/*c*

The full symbols for the three cell choices (rows) and the three unique axes (columns) read

*C*12/*c*1	*A*12/*n*1	*I*12/*a*1
*A*112/*a*	*B*112/*n*	*I*112/*b*
*B*2/*b*11	*C*2/*n*11	*I*2/*c*11.

Application of the priority rule would have resulted in the following symbols:

*C*12/*c*1	*A*12/*a*1	*I*12/*a*1
*A*112/*a*	*B*112/*b*	*I*112/*a*
*B*2/*b*11	*C*2/*c*11	*I*2/*b*11.

Here, the transformation properties are obscured.

Comparison with earlier editions of International Tables. In *IT* (1935), each monoclinic space group was presented in one description only, with *b* as the unique axis. Hence, only one short Hermann–Mauguin symbol was needed.

In *IT* (1952), the *c*-axis setting (first setting) was newly introduced, in addition to the *b*-axis setting (second setting). This extension was based on a decision of the Stockholm General Assembly of the International Union of Crystallography in 1951 [*cf. Acta Cryst.* (1951), **4**, 569 and *Preface* to *IT* (1952)]. According to this decision, the *b*-axis setting should continue to be accepted as standard for morphological and structural studies. The two settings led to the introduction of *full* Hermann–Mauguin symbols for *all* 13 monoclinic space groups (*e.g.* $P12_1/c1$ and $P112_1/b$) and of two different *standard short* symbols (*e.g.* $P2_1/c$ and $P2_1/b$) for the *eight* space groups with centred lattices or glide planes [*cf.* p. 545 of *IT* (1952)]. In the present volume (as in the previous editions of this series), only one of these standard short symbols is retained (see above and Section 2.1.3.3).

The *c*-axis setting (primed labels) was obtained from the *b*-axis setting (unprimed labels) by the following transformation:

$$(\mathbf{a}', \mathbf{b}', \underline{\mathbf{c}}') = (\mathbf{a}, \underline{\mathbf{b}}, \mathbf{c}) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix} = (\mathbf{a}, \mathbf{c}, \underline{\bar{\mathbf{b}}}).$$

This corresponds to an interchange of two labels and not to the more logical cyclic permutation, as used in all editions of this series. The reason for this particular transformation was to obtain short space-group symbols that indicate the setting unambiguously; thus the lattice letters were chosen as C (b-axis setting) and B (c-axis setting). The use of A in either case would not have distinguished between the two settings [*cf.* pp. 7, 55 and 543 of *IT* (1952); see also Table 2.1.3.12].

As a consequence of the different transformations between b- and c-axis settings in *IT* (1952) and in this volume (and all editions of this series), some space-group symbols have changed. This is apparent from a comparison of pairs such as $P12_1/c1$ & $P112_1/b$ and $C12/c1$ & $B112/b$ in *IT* (1952) with the corresponding pairs in this volume, $P12_1/c1$ & $P112_1/a$ and $C12/c1$ & $A112/a$. The symbols with B-centred cells appear now for cell choice 2, as can be seen from Table 2.1.3.12.

Selection of monoclinic cell. In practice, the selection of the (right-handed) unit cell of a monoclinic crystal can be approached in three ways, whereby the axes refer to the b-unique setting; for c unique similar considerations apply:

(i) Irrespective of their lengths, the basis vectors are chosen such that, in Fig. 2.1.3.12, one obtains $\mathbf{c} = \mathbf{e}$, $\mathbf{a} = \mathbf{f}$ and $\mathbf{b}$ normal to $\mathbf{a}$ and $\mathbf{c}$ pointing upwards. This corresponds to a selection of cell choice 1. It ensures that the crystal structure can always be referred directly to the description and the space-group symbol in *IT* (1935) and *IT* (1952). However, this is at the expense of possibly using a non-reduced and, in many cases, even a very awkward cell.

(ii) Selection of the reduced mesh, *i.e.* the shortest two translation vectors in the monoclinic plane are taken as axes and labelled $\mathbf{a}$ and $\mathbf{c}$, with either $a < c$ or $c < a$. This results with equal probability in one of the three cell choices described in the present volume.

(iii) Selection of the cell on special grounds, *e.g.* to compare the structure under consideration with another related crystal structure. This may result again in a non-reduced cell and it may even necessitate use of the a-axis setting. In all these cases, the coordinate system chosen should be carefully explained in the description of the structure.

2.1.3.16. Crystallographic groups in one dimension

In one dimension, only one crystal family, one crystal system and one Bravais lattice exist. No name or common symbol is required for any of them. All one-dimensional lattices are primitive, which is symbolized by the script letter $\mathscr{p}$; *cf.* Table 2.1.1.1.

There occur two types of one-dimensional point groups, 1 and $m \equiv \bar{1}$. The latter contains reflections through a point (reflection point or mirror point). This operation can also be described as inversion through a point, thus $m \equiv \bar{1}$ for one dimension; *cf.* Section 2.1.2.

Two types of line groups (one-dimensional space groups) exist, with Hermann–Mauguin symbols $\mathscr{p}1$ and $\mathscr{p}m \equiv \mathscr{p}\bar{1}$, which are illustrated in Fig. 2.1.3.13. Line group $\mathscr{p}1$, which consists of one-dimensional translations only, has merely one (general) position with coordinate x. Line group $\mathscr{p}m$ consists of one-dimensional translations and reflections through points. It has one general and two special positions. The coordinates of the general position are x and $\bar{x}$; the coordinate of one special position is 0, that of the other $\frac{1}{2}$. The site symmetries of both special positions are $m \equiv \bar{1}$. For $\mathscr{p}1$, the origin is arbitrary, for $\mathscr{p}m$ it is at a reflection point.

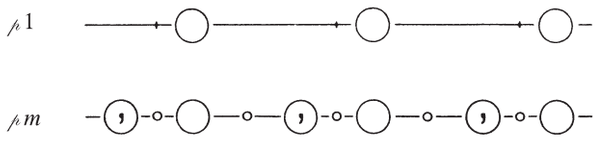


Figure 2.1.3.13
The two line groups (one-dimensional space groups). Small circles are reflection points; large circles represent the general position; in line group $\mathscr{p}1$, the vertical bars are the origins of the unit cells.

The one-dimensional *point groups* are of interest as 'edge symmetries' of two-dimensional 'edge forms'; they are listed in Table 3.2.3.1. The one-dimensional *space groups* occur as projection and section symmetries of crystal structures.

2.1.4. Computer production of the space-group tables

By P. Konstantinov and K. Momma

The space-group tables for the first (1983) edition of Volume A were produced and typeset by a computer-aided process as described by Fokkema (1983). However, the computer programs used and the data files were then lost. All corrections in the subsequent three editions were done by photocopying and 'cut-and-paste' work based on the printed version of the book.

Hence, in October 1997, a new project for the electronic production of the fifth edition of Volume A of *International Tables for Crystallography* was started. Part of this project concerned the computer generation of the plane- and space-group tables [Parts 6 and 7 of *IT* A (2002)], excluding the space-group diagrams. The aim was to be able to produce PostScript and Portable Document Format (PDF) documents that could be used for printing and displaying the tables. The layout of the tables had to follow exactly that of the previous editions of Volume A. Having the space-group tables in electronic form opened the way for easy corrections and modifications of later editions and made possible the online edition of Volume A in 2006 (http://it.iucr.org/A/). Although the plane- and space-group data were encoded in a format designed for printing, they were later machine-read and transformed to other electronic formats, and were incorporated into the data files on which the Symmetry Database in the online version of *International Tables for Crystallography* (http://it.iucr.org/resources/symmetrydatabase/) and the online services offered by the Bilbao Crystallographic Server (http://www.cryst.ehu.es/) are based.

The LaTeX document preparation system (Lamport, 1994), which is based on the TeX typesetting software, was used for the preparation of these tables. It was chosen because of its high versatility and general availability on almost any computer platform. It is also worth noting the longevity of the system. Even though the hardware and operating system software used almost 20 years ago, when the project began, are now obsolete, the software is still available on all major modern computer systems. All the material – LaTeX code and data – created for the fifth edition of 2002 was re-used in the preparation of the current edition with only small changes concerning the presentation.

A separate file was created for each plane and space group and each setting. These data files contain the information listed in the plane- and space-group tables and are encoded using standard LaTeX constructs. As is customary, these specially designed commands and environments are defined in a separate package

file, which essentially contains routines, called macros, that control the typographical layout of the data. Thus, the main principle of LaTeX – that of keeping content and presentation separate – was followed as closely as possible.

The final typesetting of all the plane- and space-group tables was done by running a single computer job. References in the tables from one page to another are automatically computed. The result is a PostScript file which can be fed to a laser printer or other printing or typesetting equipment. It can also be easily converted to a PDF file. It is also possible to generate the output for just one group, as accessed in the online edition, or a series of groups.

The different types of data in the LaTeX files were either keyed by hand or computer generated, and were additionally checked by specially written programs. The preparation of the data files can be summarized as follows:

Headline, *Origin*, *Asymmetric unit*: hand keyed.

Symmetry operations: partly created by a computer program. The algorithm for the derivation of symmetry operations from their matrix representation is similar to that described in the literature (*cf.* Section 1.2.2; see also Hahn & Wondratschek, 1994). The data were additionally checked by automatic comparison with the output of the computer program *SPACER* (Stróż, 1997).

Generators: transferred automatically from the data for Volume A1 of *International Tables for Crystallography* (2010), hereafter referred to as *IT* A1.

General positions: created by a program. The algorithm uses the well known generating process for space groups based on their solvability property (*cf.* Section 1.4.3).

Special positions: The first representatives of the Wyckoff positions were typed in by hand. The Wyckoff letters are assigned automatically by the TeX macros according to the order of appearance of the special positions in the data file. The multiplicity of the position, the oriented site-symmetry symbol and the rest of the representatives of the Wyckoff position were generated by a program. Again, the data were compared with the results of the program *SPACER*.

Reflection conditions: hand keyed. A program for automatic checking of the special-position coordinates and the corresponding reflection conditions with h, k, l ranging from -20 to 20 was developed.

Symmetry of special projections: hand keyed.

Maximal subgroups and minimal supergroups: this information appeared in the fifth revised edition of Volume A, as in the previous editions. Most of the data were automatically transferred from the data files used for the production of *IT* A1. The macros for typesetting these data were re-implemented to obtain exactly the layout of Volume A. For the current edition these data have been omitted by redefining the macros to ignore the content, which is still present in the data files.

The symmetry-element diagrams were scanned and processed in the IUCr Editorial Office in Chester.

In the first edition of *IT* A published in 1983, the general-position diagrams of the cubic groups presented in the 1935 edition of *Internationale Tabellen zur Bestimmung von Kristallstrukturen* were replaced by small stereodiagrams. At that time, such stereodiagrams were probably the easiest way to allow three-dimensional visualization, and the same stereodiagrams were reproduced in the following editions. However, the sizes of the stereodiagrams were limited by the page size, so they were very small, and they also lacked any indication of general-position 'enantiomorph' points. The situation has changed a lot since then and three-dimensional visualization of the general positions is easily achieved with structure-drawing programs. Therefore, in this sixth edition, new general-position diagrams of the cubic groups, which are similar to those of the non-cubic groups, were created with a focus on better two-dimensional representation in print.

The new diagrams were created by K. Momma using the computer program *VESTA* (Momma & Izumi, 2011), which was extended for this purpose. The diagrams that were generated were carefully checked by comparing them with the original diagrams in the 1935 edition. The coordinates of general positions are slightly different from those used in the original diagrams and were chosen so that the general positions overlap as little as possible in the two-dimensional orthogonal projection of the diagrams. The coordinates of general positions used are:

(i) 0.0375, 0.1125, 0.098 for space-group Nos. 198, 199, 205, 206, 212, 213, 214, 220 and 230;
(ii) 0.065, 0.12, 0.048 for the second diagrams of space-group Nos. 212, 214 and 230;
(iii) 0.435, 0.38, 0.452 for the second diagram of space-group No. 213;
(iv) 0.31, 0.095, 0.21 for the second diagram of space-group No. 220; and
(v) $0.048x$, $0.12y$, $0.089z$ for the remaining space groups, where x, y, z is the first coordinate triplet of the highest symmetry Wyckoff position of the space group.

In addition, three-dimensional-style tilted general-position diagrams were created by *VESTA* for each of the ten space groups of the $m\bar{3}m$ crystal class. These diagrams can be reproduced and visualized in three dimensions using *VESTA*. They were provided in the form of Portable Network Graphics (PNG) raster images and were included in the page layout of the space-group tables with some scaling and cropping.

The preparation of the plane- and space-group tables was carried out on various computer platforms in Sofia, Bilbao, Karlsruhe, Tsukuba and Chester. The development of the computer programs and the layout macros in the LaTeX package file, and the preparation of the diagrams were done in parallel by different members of the team, which included Asen Kirov (Sofia), Eli Kroumova (Bilbao), Koichi Momma, Preslav Konstantinov and Mois Aroyo, and staff at the Editorial Office in Chester.

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2.2. THE 17 PLANE GROUPS (TWO-DIMENSIONAL SPACE GROUPS)

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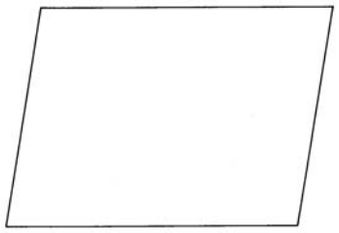
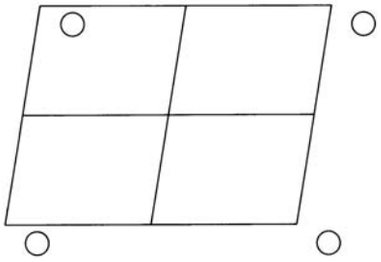
$p\,1$ 1 Oblique

No. 1 $p\,1$ Patterson symmetry $p\,2$





Origin arbitrary

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1$

Symmetry operations

(1) 1

Generators selected (1); $t(1,0)$; $t(0,1)$

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	Reflection conditions
			General:
1	*a* 1	(1) x,y	no conditions

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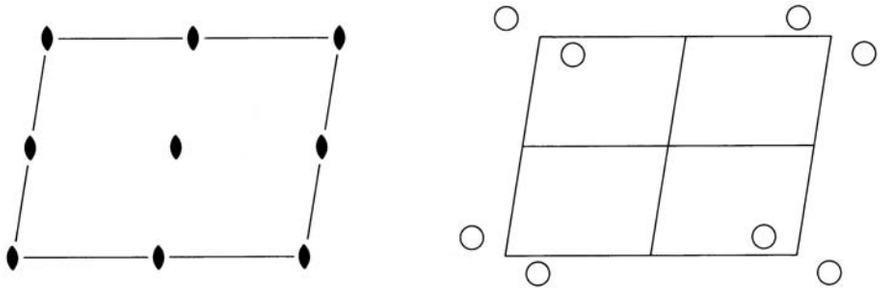
Oblique 2 $p2$

Patterson symmetry $p2$ $p2$ No. 2



Origin at 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (2) 2 0,0

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	*e*	1	(1) x,y	(2) $\bar{x},\bar{y}$	no conditions
					Special: no extra conditions
1	*d*	2	$\frac{1}{2},\frac{1}{2}$		
1	*c*	2	$\frac{1}{2},0$		
1	*b*	2	$0,\frac{1}{2}$		
1	*a*	2	$0,0$		

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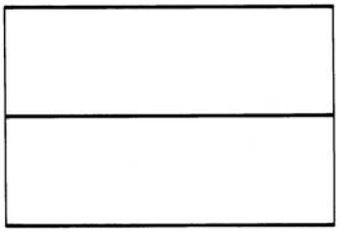
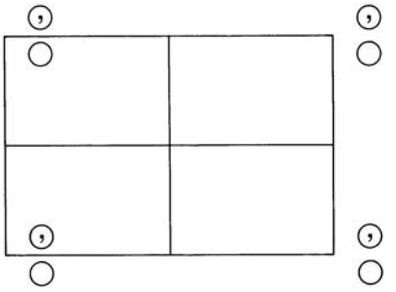
p m *m* Rectangular

No. 3 *p* 1 *m* 1 Patterson symmetry *p* 2 *m m*





Origin on *m*

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (2) *m* 0, *y*

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	*c*	1	(1) *x*, *y*	(2) $\bar{x}, y$	no conditions
					Special: no extra conditions
1	*b*	. *m* .	$\frac{1}{2}, y$		
1	*a*	. *m* .	0, *y*		

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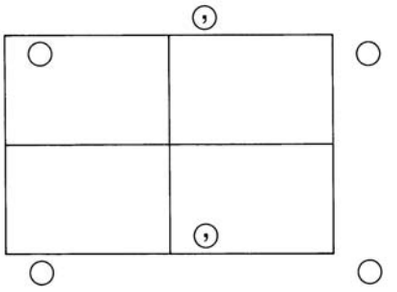
Rectangular m $p\,g$

Patterson symmetry $p\,2\,m\,m$ $p\,1\,g\,1$ No. 4



Origin on g

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (2) b $0, y$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x, y	(2) $\bar{x}, y+\frac{1}{2}$	$0k$: $k = 2n$

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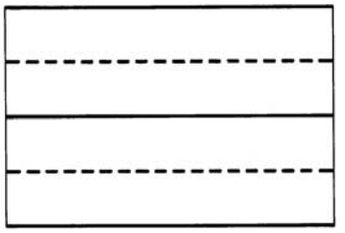
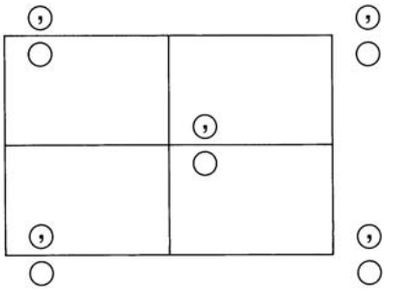
cm *m* Rectangular

No. 5 *c*1*m*1 Patterson symmetry *c*2*mm*





Origin on *m*

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0)+$ set

(1) 1 (2) m $0,y$

For $(\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2})$ (2) b $\frac{1}{4},y$

Generators selected (1); $t(1,0)$; $t(0,1)$; $t(\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0)+$	$(\frac{1}{2},\frac{1}{2})+$	Reflection conditions
			General:
4 b 1	(1) x,y	(2) $\bar{x},y$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
			Special: no extra conditions
2 a $.m.$	$0,y$		

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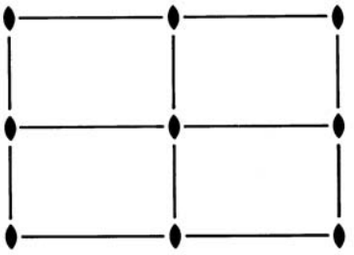
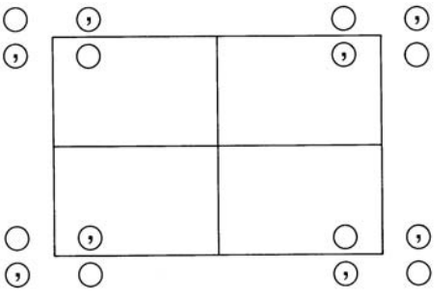
Rectangular $2mm$ $p2mm$

Patterson symmetry $p2mm$ $p2mm$ No. 6





Origin at $2mm$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0$ (3) m $0,y$ (4) m $x,0$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	i	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x},y$	(4) $x,\bar{y}$	no conditions
							Special: no extra conditions
2	h	$.m.$	$\frac{1}{2},y$	$\frac{1}{2},\bar{y}$			
2	g	$.m.$	$0,y$	$0,\bar{y}$			
2	f	$..m$	$x,\frac{1}{2}$	$\bar{x},\frac{1}{2}$			
2	e	$..m$	$x,0$	$\bar{x},0$			
1	d	$2mm$	$\frac{1}{2},\frac{1}{2}$				
1	c	$2mm$	$\frac{1}{2},0$				
1	b	$2mm$	$0,\frac{1}{2}$				
1	a	$2mm$	$0,0$				

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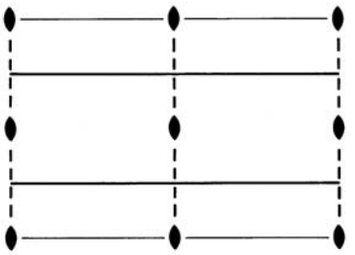
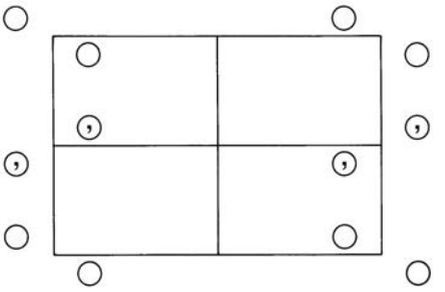
$p2mg$ $2mm$ Rectangular

No. 7 $p2mg$ Patterson symmetry $p2mm$





Origin at $2\,1\,g$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0$ (3) m $\frac{1}{4},y$ (4) a $x,0$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x}+\frac{1}{2},y$	(4) $x+\frac{1}{2},\bar{y}$	$h0$: $h = 2n$
							Special: as above, plus
2	c	$.m.$	$\frac{1}{4},y$	$\frac{3}{4},\bar{y}$			no extra conditions
2	b	$2..$	$0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$			hk: $h = 2n$
2	a	$2..$	$0,0$	$\frac{1}{2},0$			hk: $h = 2n$

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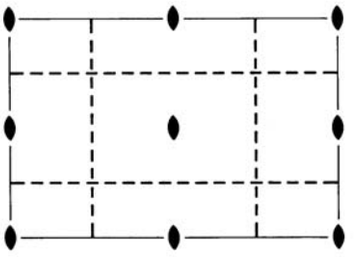
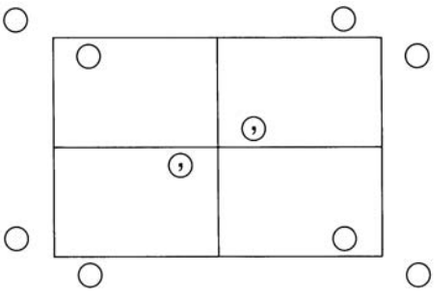
Rectangular $2mm$ $p2gg$

Patterson symmetry $p2mm$ $p2gg$ No. 8





Origin at 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0$ (3) b $\frac{1}{4},y$ (4) a $x,\frac{1}{4}$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
4 c 1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$h0$: $h=2n$ $0k$: $k=2n$
		Special: as above, plus
2 b 2 . .	$\frac{1}{2},0$ $0,\frac{1}{2}$	hk: $h+k=2n$
2 a 2 . .	$0,0$ $\frac{1}{2},\frac{1}{2}$	hk: $h+k=2n$

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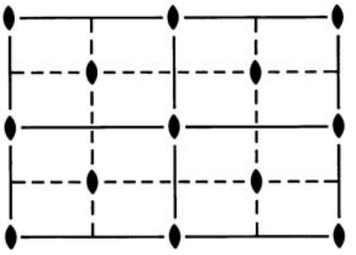
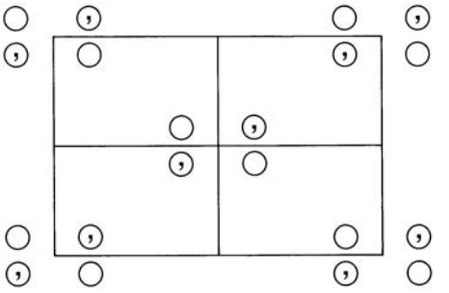
$c2mm$ $2mm$ Rectangular

No. 9 $c2mm$ Patterson symmetry $c2mm$





Origin at $2mm$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}$

Symmetry operations

For $(0,0)+$ set

(1) 1 (2) 2 $0,0$ (3) m $0,y$ (4) m $x,0$

For $(\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2})$ (2) 2 $\frac{1}{4},\frac{1}{4}$ (3) b $\frac{1}{4},y$ (4) a $x,\frac{1}{4}$

Generators selected (1); $t(1,0)$; $t(0,1)$; $t(\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0)+$	Coordinates $(\frac{1}{2},\frac{1}{2})+$		Reflection conditions
						General:
8	f	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x},y$ (4) $x,\bar{y}$	hk: $h+k=2n$ $h0$: $h=2n$ $0k$: $k=2n$
						Special: as above, plus
4	e	$.m.$	$0,y$	$0,\bar{y}$		no extra conditions
4	d	$..m$	$x,0$	$\bar{x},0$		no extra conditions
4	c	$2..$	$\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4}$		hk: $h=2n$
2	b	$2\,m\,m$	$0,\frac{1}{2}$			no extra conditions
2	a	$2\,m\,m$	$0,0$			no extra conditions

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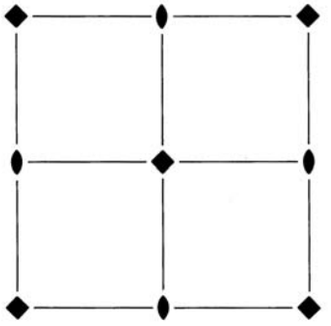
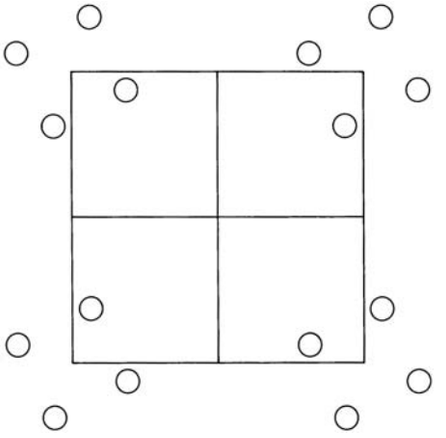
Square 4 *p*4

Patterson symmetry *p*4 *p*4 No. 10





Origin at 4

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 0,0 (3) 4^+ 0,0 (4) 4^- 0,0

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*d*	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{y},x$	(4) $y,\bar{x}$	no conditions
							Special:
2	*c*	2 . .	$\frac{1}{2},0$	$0,\frac{1}{2}$			*hk*: $h+k=2n$
1	*b*	4 . .	$\frac{1}{2},\frac{1}{2}$				no extra conditions
1	*a*	4 . .	0,0				no extra conditions

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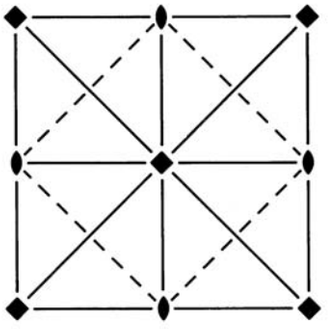
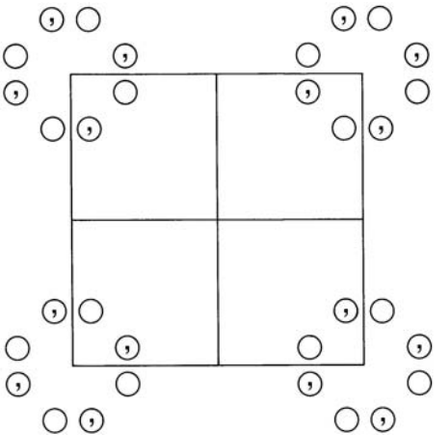
$p4mm$ $4mm$ Square

No. 11 $p4mm$ Patterson symmetry $p4mm$





Origin at $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $x \le y$

Symmetry operations

(1) 1 (2) 2 0,0 (3) 4^+ 0,0 (4) 4^- 0,0
(5) m 0,y (6) m x,0 (7) m x,x (8) m $x,\bar{x}$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y (5) $\bar{x},y$	(2) $\bar{x},\bar{y}$ (6) $x,\bar{y}$	(3) $\bar{y},x$ (7) y,x	(4) $y,\bar{x}$ (8) $\bar{y},\bar{x}$	no conditions
							Special:
4	f	. . m	x,x	$\bar{x},\bar{x}$	$\bar{x},x$	$x,\bar{x}$	no extra conditions
4	e	. m .	$x,\frac{1}{2}$	$\bar{x},\frac{1}{2}$	$\frac{1}{2},x$	$\frac{1}{2},\bar{x}$	no extra conditions
4	d	. m .	$x,0$	$\bar{x},0$	$0,x$	$0,\bar{x}$	no extra conditions
2	c	2 m m .	$\frac{1}{2},0$	$0,\frac{1}{2}$			hk: $h+k=2n$
1	b	4 m m	$\frac{1}{2},\frac{1}{2}$				no extra conditions
1	a	4 m m	0,0				no extra conditions

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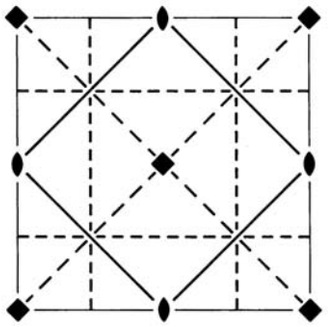
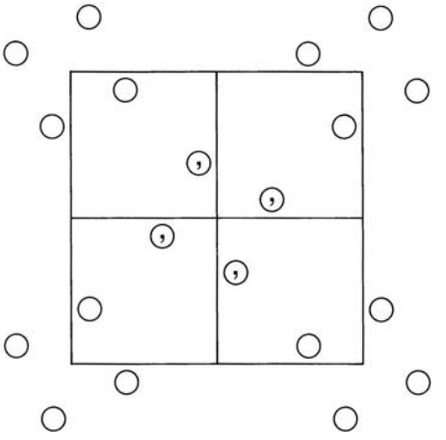
Square $4mm$ $p4gm$

Patterson symmetry $p4mm$ $p4gm$ No. 12





Origin at 4 1 g

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 0,0	(3) 4^+ 0,0	(4) 4^- 0,0
(5) b $\frac{1}{4},y$	(6) a $x,\frac{1}{4}$	(7) $g(\frac{1}{2},\frac{1}{2})$ x,x	(8) m $x+\frac{1}{2},\bar{x}$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{y},x$	(4) $y,\bar{x}$	$h0$: $h = 2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$0k$: $k = 2n$
							Special: as above, plus
4	c	. . m	$x,x+\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x$	$x+\frac{1}{2},\bar{x}$	no extra conditions
2	b	2 . mm	$\frac{1}{2},0$	$0,\frac{1}{2}$			hk: $h+k = 2n$
2	a	4 . .	0,0	$\frac{1}{2},\frac{1}{2}$			hk: $h+k = 2n$

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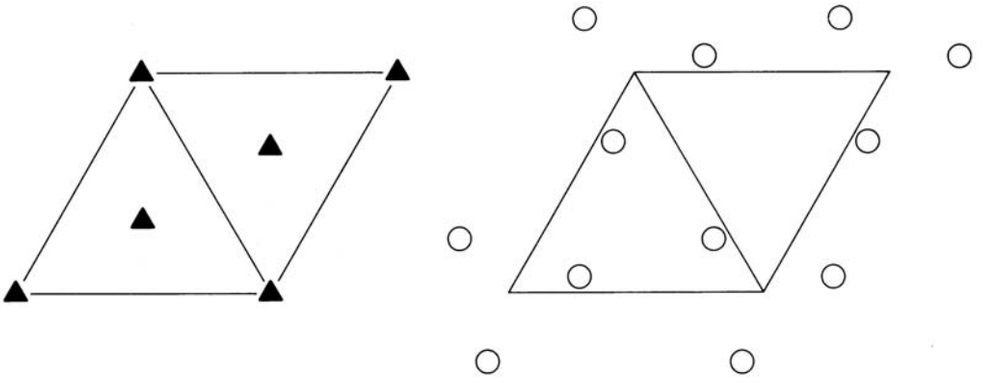
$p3$ 3 Hexagonal

No. 13 $p3$ Patterson symmetry $p6$



Origin at 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$
Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0$ (3) 3^- $0,0$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	d	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$	no conditions
						Special: no extra conditions
1	c	3 . .	$\frac{2}{3},\frac{1}{3}$			
1	b	3 . .	$\frac{1}{3},\frac{2}{3}$			
1	a	3 . .	$0,0$			

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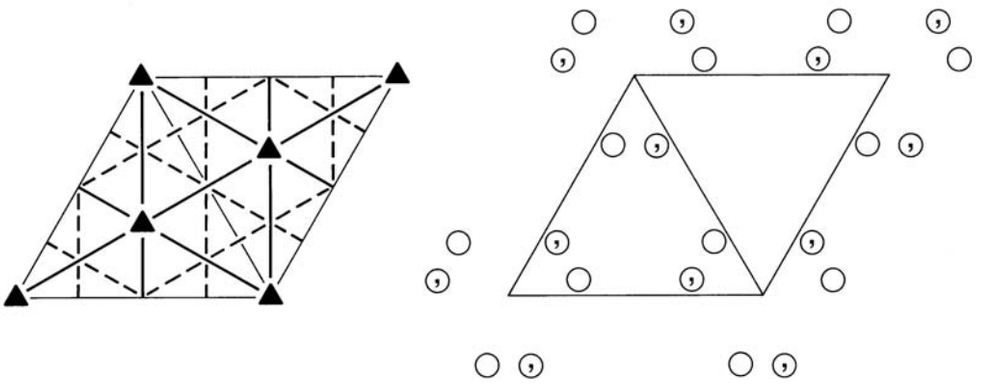
Hexagonal $3m$ $p3m1$

Patterson symmetry $p6mm$ $p3m1$ No. 14



Origin at $3m1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$

Symmetry operations

(1) 1 (2) 3^+ $0,0$ (3) 3^- $0,0$
(4) m $x,\bar{x}$ (5) m $x,2x$ (6) m $2x,x$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 e 1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$	no conditions
	(4) $\bar{y},\bar{x}$	(5) $\bar{x}+y,y$	(6) $x,x-y$	
				Special: no extra conditions
3 d $.m.$	$x,\bar{x}$	$x,2x$	$2\bar{x},\bar{x}$	
1 c $3m.$	$\frac{2}{3},\frac{1}{3}$			
1 b $3m.$	$\frac{1}{3},\frac{2}{3}$			
1 a $3m.$	$0,0$			

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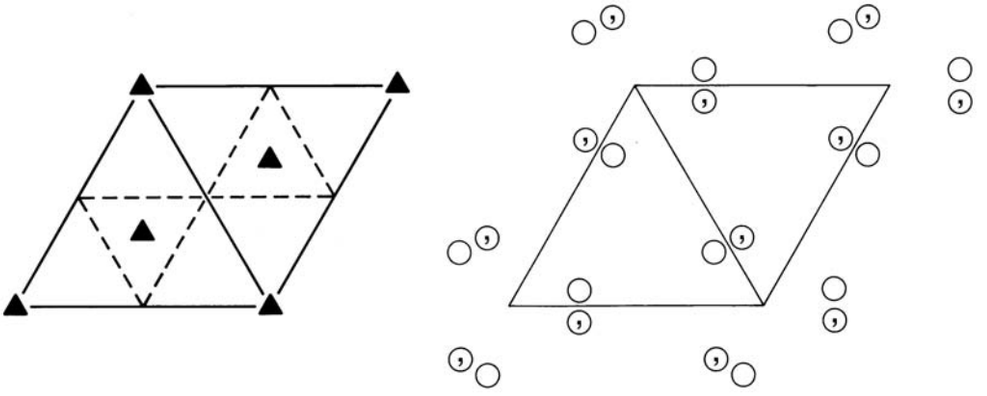
$p\,3\,1\,m$ $3\,m$ Hexagonal

No. 15 $p\,3\,1\,m$ Patterson symmetry $p\,6\,m\,m$



Origin at $3\,1\,m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x, x)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ 0,0 (3) 3^- 0,0
(4) m x,x (5) m $x,0$ (6) m $0,y$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
			(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$	General:
6	d	1	(4) y,x	(5) $x-y,\bar{y}$	(6) $\bar{x},\bar{x}+y$	no conditions
						Special: no extra conditions
3	c	$.\,.\,m$	$x,0$	$0,x$	$\bar{x},\bar{x}$	
2	b	$3\,.\,.$	$\frac{1}{3},\frac{2}{3}$	$\frac{2}{3},\frac{1}{3}$		
1	a	$3\,.\,m$	$0,0$			

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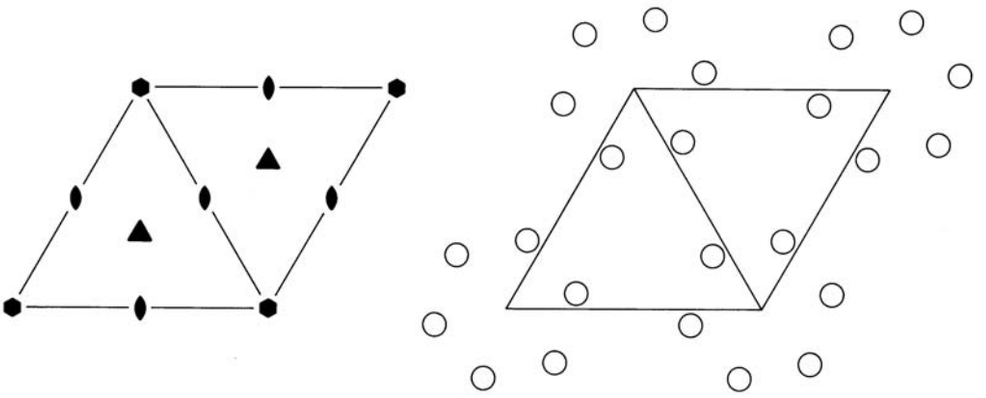
Hexagonal 6 *p*6

Patterson symmetry *p*6 *p*6 No. 16



Origin at 6

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x, x)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ 0,0 (3) 3^- 0,0
(4) 2 0,0 (5) 6^- 0,0 (6) 6^+ 0,0

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*d*	1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$	no conditions
			(4) $\bar{x},\bar{y}$	(5) $y,\bar{x}+y$	(6) $x-y,x$	
						Special: no extra conditions
3	*c*	2 . .	$\frac{1}{2},0$	$0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$	
2	*b*	3 . .	$\frac{1}{3},\frac{2}{3}$	$\frac{2}{3},\frac{1}{3}$		
1	*a*	6 . .	0,0			

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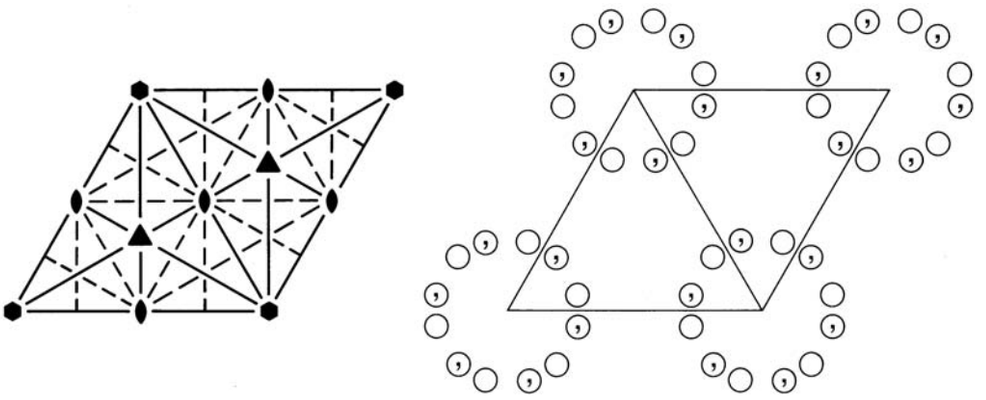
$p6mm$ $6mm$ Hexagonal

No. 17 $p6mm$ Patterson symmetry $p6mm$



Origin at $6mm$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$

Symmetry operations

(1) 1	(2) 3^+ 0,0	(3) 3^- 0,0
(4) 2 0,0	(5) 6^- 0,0	(6) 6^+ 0,0
(7) m $x,\bar{x}$	(8) m $x,2x$	(9) m $2x,x$
(10) m x,x	(11) m $x,0$	(12) m $0,y$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
							General:
12 f 1	(1) x,y	(2) $\bar{y},x-y$	(3) $\bar{x}+y,\bar{x}$				no conditions
	(4) $\bar{x},\bar{y}$	(5) $y,\bar{x}+y$	(6) $x-y,x$				
	(7) $\bar{y},\bar{x}$	(8) $\bar{x}+y,y$	(9) $x,x-y$				
	(10) y,x	(11) $x-y,\bar{y}$	(12) $\bar{x},\bar{x}+y$				
							Special: no extra conditions
6 e . m .	$x,\bar{x}$	$x,2x$	$2\bar{x},\bar{x}$	$\bar{x},x$	$\bar{x},2\bar{x}$	$2x,x$	
6 d . . m	$x,0$	$0,x$	$\bar{x},\bar{x}$	$\bar{x},0$	$0,\bar{x}$	x,x	
3 c 2 m m	$\frac{1}{2},0$	$0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$				
2 b 3 m .	$\frac{1}{3},\frac{2}{3}$	$\frac{2}{3},\frac{1}{3}$					
1 a 6 m m	0,0						

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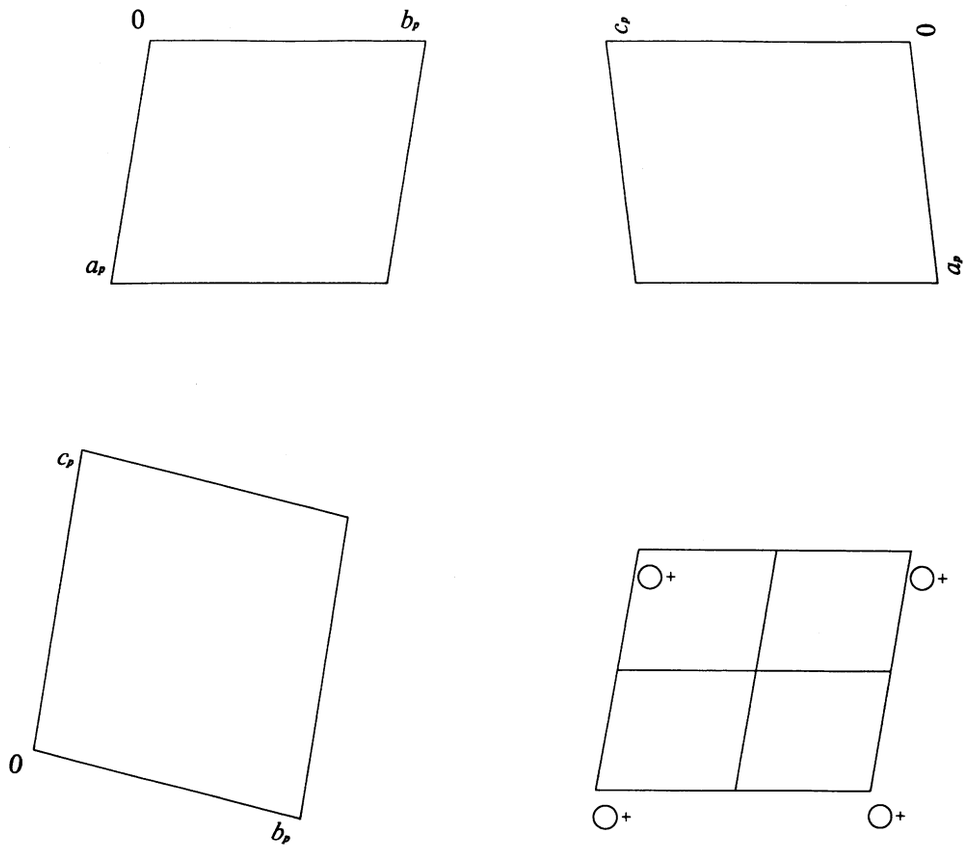
$P1$ C_1^1 1 Triclinic

No. 1 $P1$ Patterson symmetry $P\bar{1}$



Drawings for type II cell. Proper cell reduction (Section 3.1.3) gives either a type I (α, β, γ acute) or a type II (α, β, γ non-acute) cell.

Origin arbitrary

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le 1$

Symmetry operations

(1) 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
1 a 1	(1) x,y,z	no conditions

Symmetry of special projections

Along [001] $p1$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}_p$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p1$
$\mathbf{a}' = \mathbf{c}_p$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

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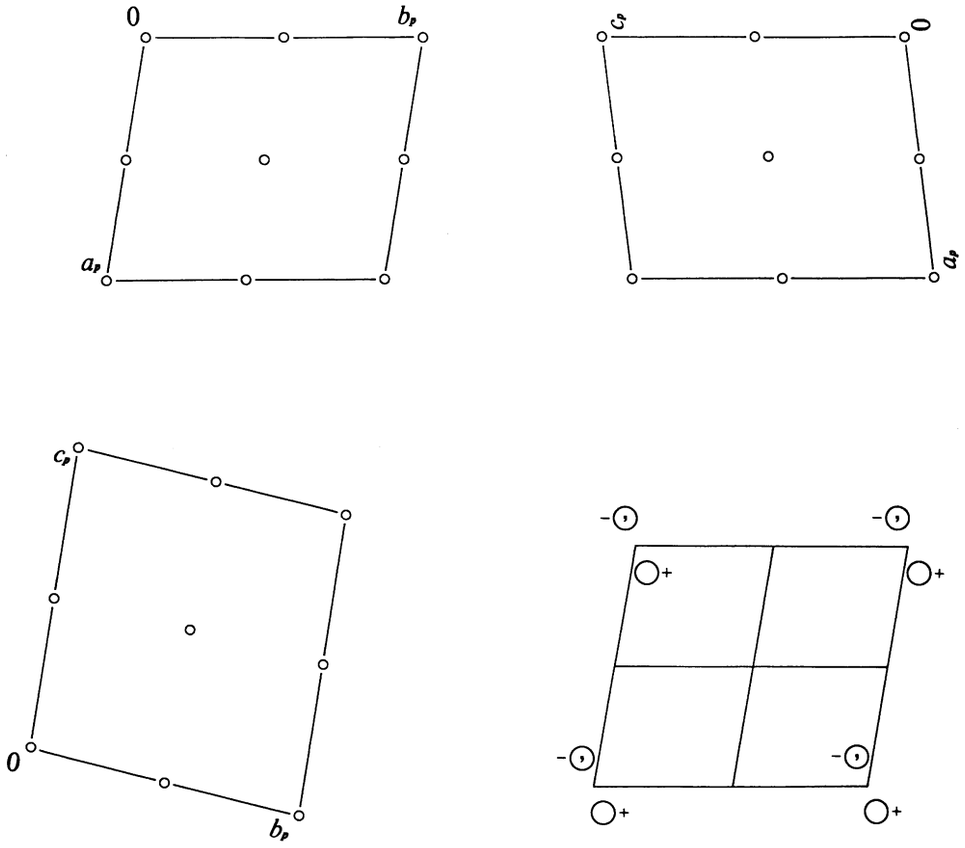
Triclinic $\bar{1}$ C_i^1 $P\bar{1}$

Patterson symmetry $P\bar{1}$ $P\bar{1}$ No. 2



Drawings for type II cell. Proper cell reduction (Section 3.1.3) gives either a type I (α, β, γ acute) or a type II (α, β, γ non-acute) cell.

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $\bar{1}$ 0,0,0

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
2	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},\bar{z}$	General: no conditions
					Special: no extra conditions
1	h	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
1	g	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$		
1	f	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$		
1	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$		
1	d	$\bar{1}$	$\frac{1}{2},0,0$		
1	c	$\bar{1}$	$0,\frac{1}{2},0$		
1	b	$\bar{1}$	$0,0,\frac{1}{2}$		
1	a	$\bar{1}$	$0,0,0$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}_p$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \mathbf{c}_p$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

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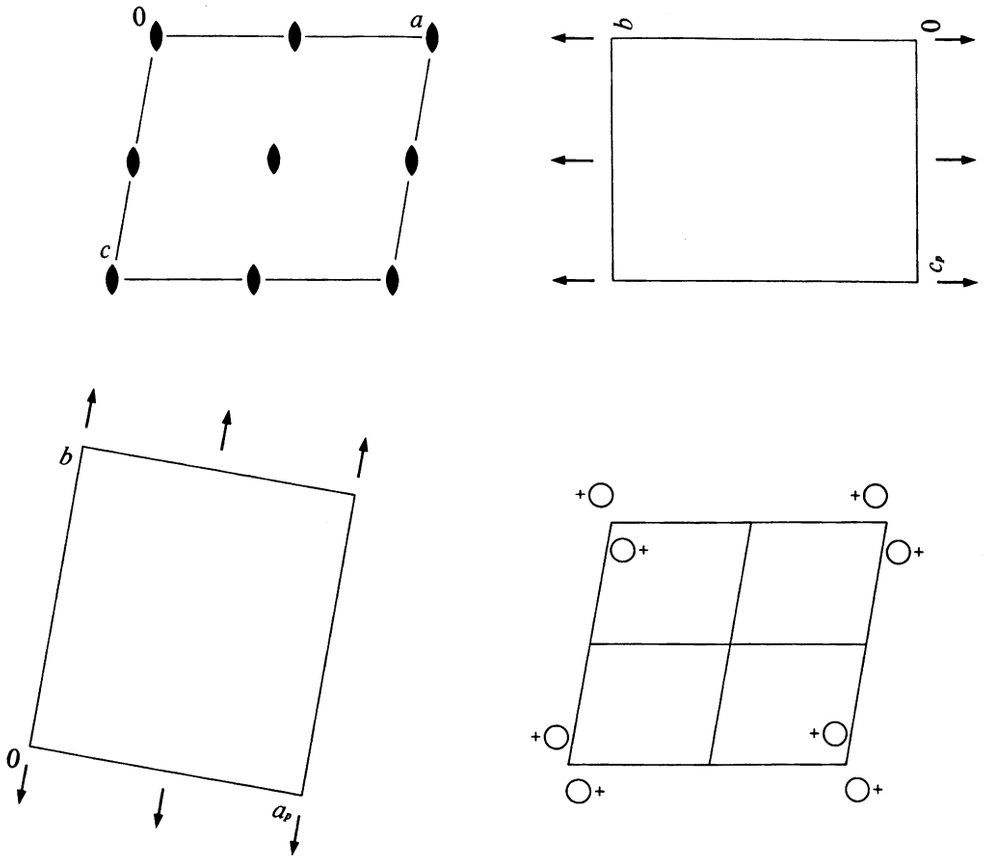
$P2$ C_2^1 2 Monoclinic

No. 3 $P121$ Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin on 2

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	e	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	no conditions
					Special: no extra conditions
1	d	2	$\frac{1}{2},y,\frac{1}{2}$		
1	c	2	$\frac{1}{2},y,0$		
1	b	2	$0,y,\frac{1}{2}$		
1	a	2	$0,y,0$		

Symmetry of special projections

Along [001] $p1m1$
$\mathbf{a}' = \mathbf{a}_p \quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}' = \mathbf{b} \quad \mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \mathbf{c} \quad \mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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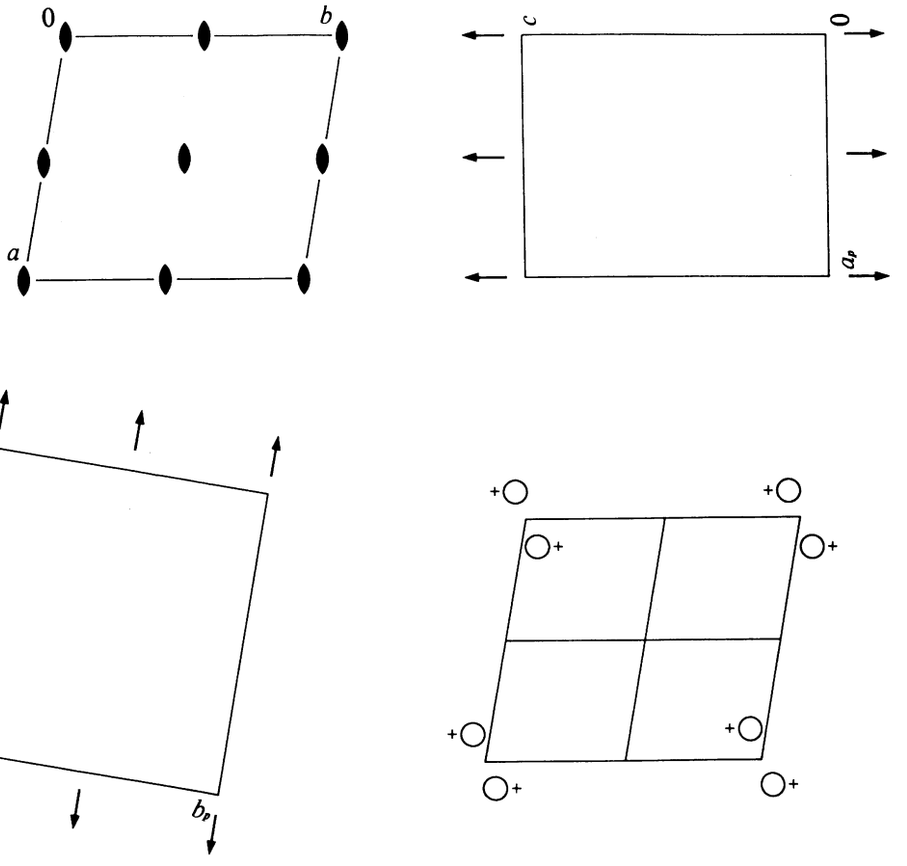


Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	no conditions
					Special: no extra conditions
1	d	2	$\frac{1}{2},\frac{1}{2},z$		
1	c	2	$0,\frac{1}{2},z$		
1	b	2	$\frac{1}{2},0,z$		
1	a	2	$0,0,z$		

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

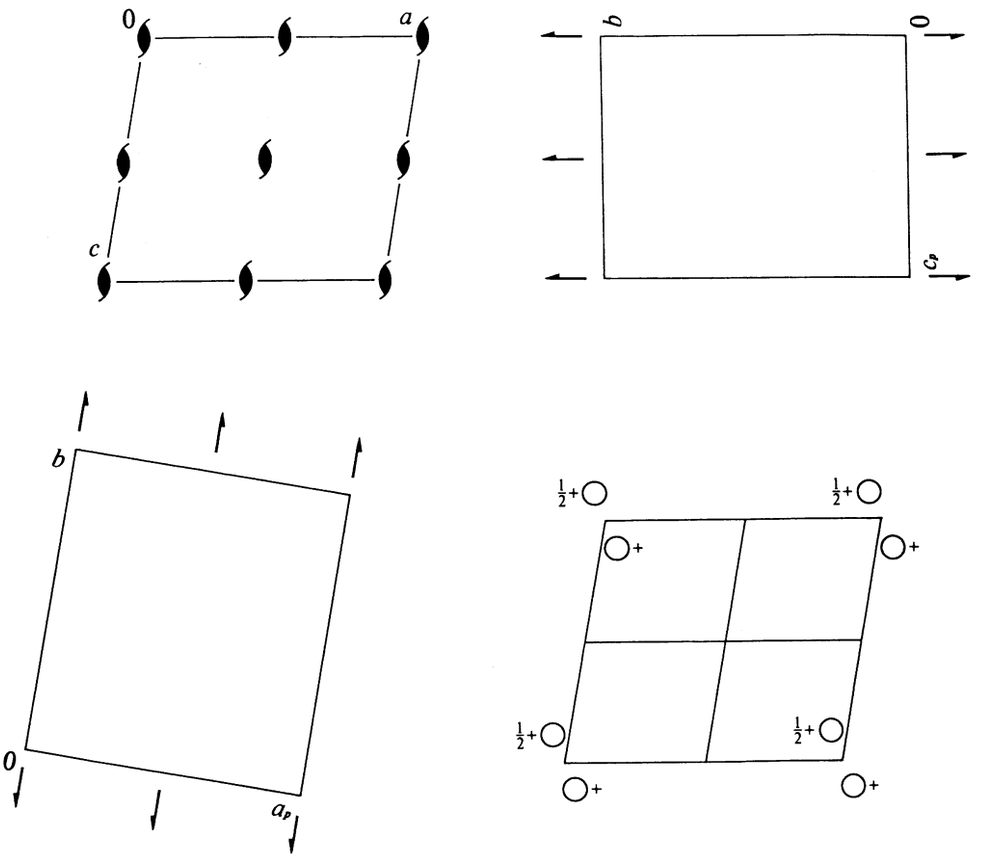
Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

$P2_1$ C_2^2 2 Monoclinic

No. 4 $P\,1\,2_1\,1$ Patterson symmetry $P\,1\,2/m\,1$

UNIQUE AXIS b



Origin on 2_1

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $\bar{x},y+\frac{1}{2},\bar{z}$	$0k0$: $k=2n$

Symmetry of special projections

Along [001] $p\,1\,g\,1$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,1\,g$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,2$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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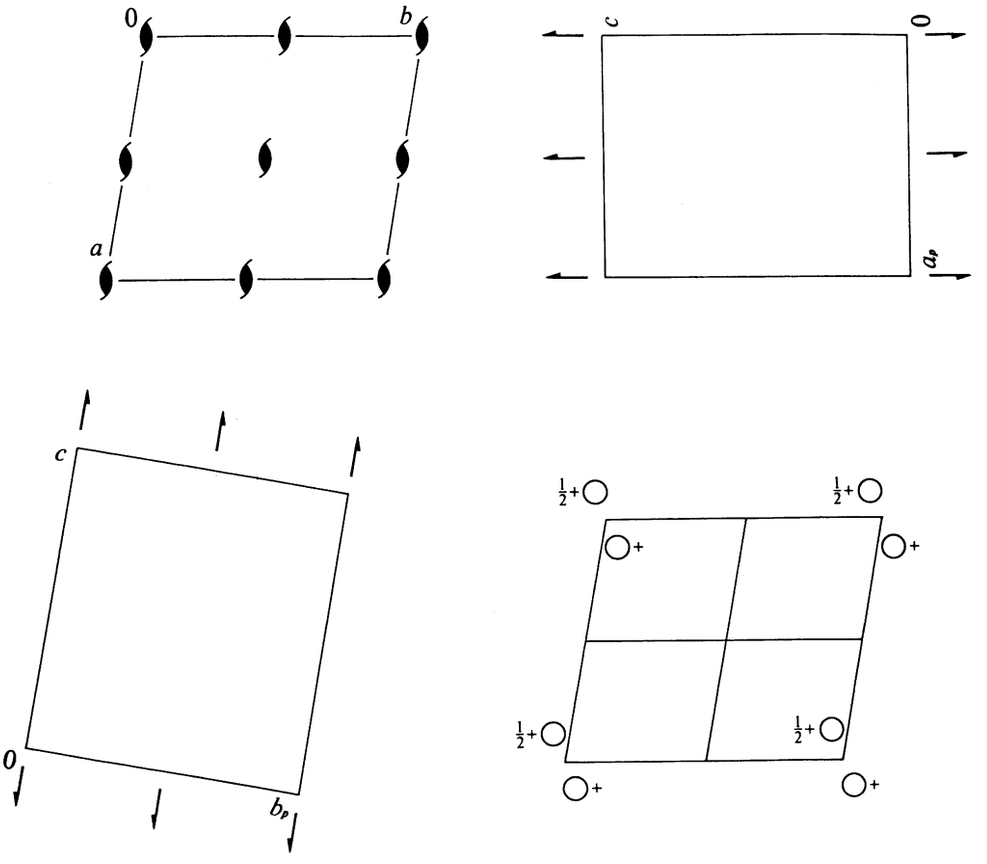


Origin on 2_1

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
2 a 1	(1) x,y,z (2) $\bar{x},\bar{y},z+\frac{1}{2}$	$00l$: $l = 2n$

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

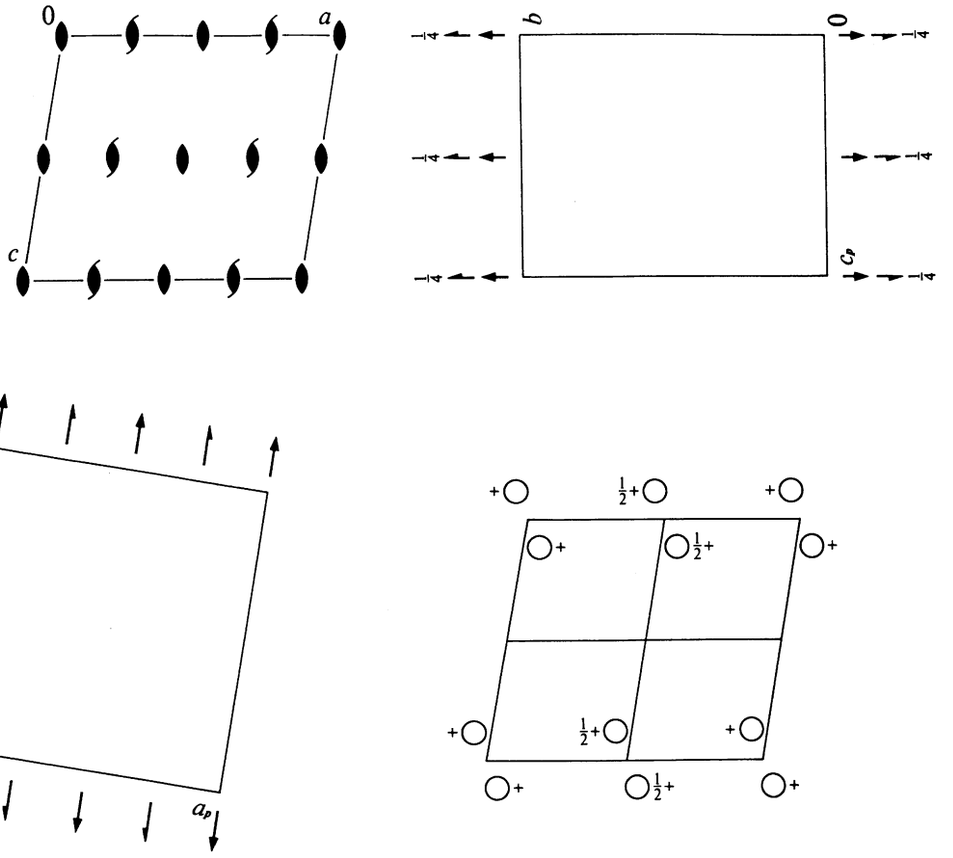
Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11g$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

$C2$ C_2^3 2 Monoclinic

No. 5 $C121$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,y,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
4	*c*	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	hkl: $h+k=2n$ $h0l$: $h=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
					Special: no extra conditions
2	*b*	2	$0,y,\frac{1}{2}$		
2	*a*	2	$0,y,0$		

Symmetry of special projections

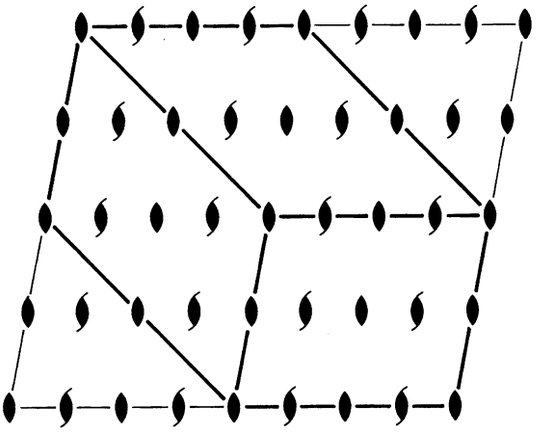
Along [001] $c\,1\,m\,1$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

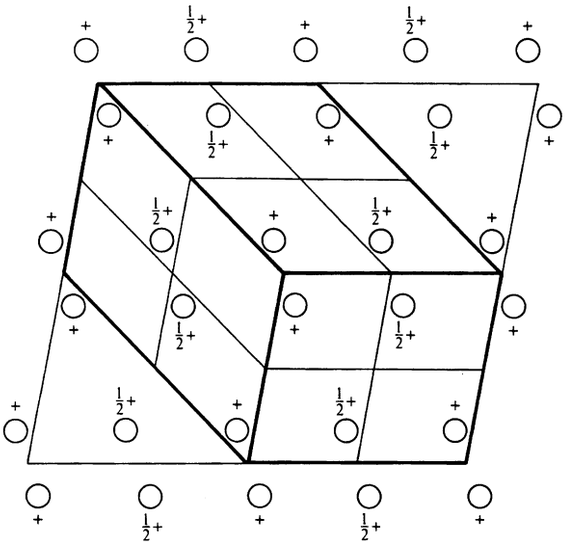
Along [100] $p\,1\,1\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,2$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

No. 5

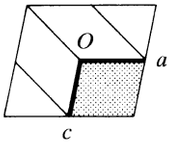
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C121$

UNIQUE AXIS b, CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

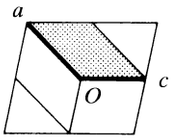
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
4	c	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	hkl: $h+k=2n$ $h0l$: $h=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
					Special: no extra conditions
2	b	2	$0,y,\frac{1}{2}$		
2	a	2	$0,y,0$		

*A*1 2 1

UNIQUE AXIS *b*, CELL CHOICE 2



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$
4	*c*	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$
2	*b*	2	$\frac{1}{2},y,\frac{1}{2}$	
2	*a*	2	$0,y,0$	

Reflection conditions

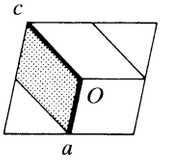
General:

hkl: $k+l=2n$
*h*0*l*: $l=2n$
0*kl*: $k+l=2n$
*hk*0: $k=2n$
0*k*0: $k=2n$
00*l*: $l=2n$

Special: no extra conditions

*I*1 2 1

UNIQUE AXIS *b*, CELL CHOICE 3



Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
4	*c*	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$
2	*b*	2	$\frac{1}{2},y,0$	
2	*a*	2	$0,y,0$	

Reflection conditions

General:

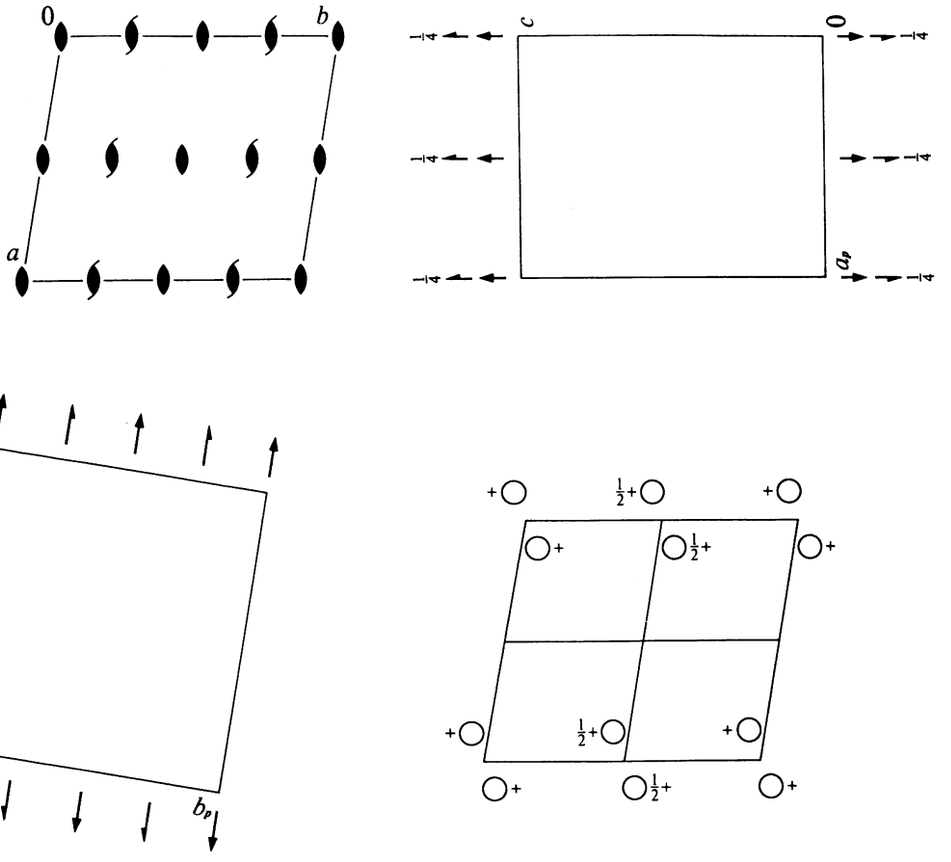
hkl: $h+k+l=2n$
*h*0*l*: $h+l=2n$
0*kl*: $k+l=2n$
*hk*0: $h+k=2n$
0*k*0: $k=2n$
*h*00: $h=2n$
00*l*: $l=2n$

Special: no extra conditions

No. 5 $A112$

Patterson symmetry $A112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	Coordinates $(0,\frac{1}{2},\frac{1}{2})+$	Reflection conditions
					General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl: $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	b	2	$\frac{1}{2},0,z$		
2	a	2	$0,0,z$		

Symmetry of special projections

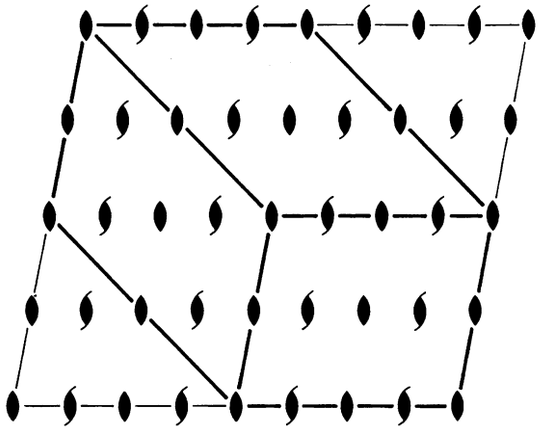
Along [001] $p2$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

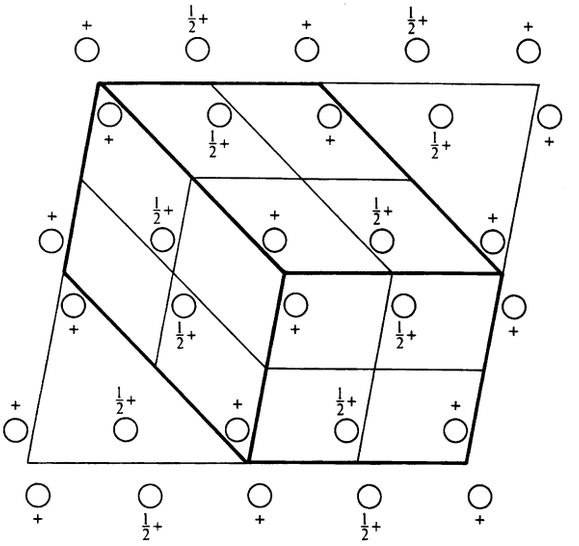
Along [100] $c1m1$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

No. 5

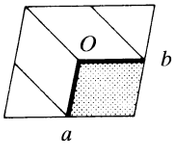
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A112$

UNIQUE AXIS c, CELL CHOICE 1



Origin on 2

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

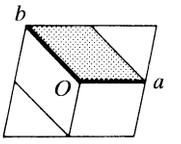
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl: $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
2	b	2	$\frac{1}{2},0,z$		Special: no extra conditions
2	a	2	$0,0,z$		

*B*112

UNIQUE AXIS *c*, CELL CHOICE 2



Origin on 2

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

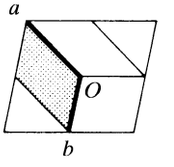
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},0,\frac{1}{2})+$	General:
4	*c*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl: $h+l=2n$ $hk0$: $h=2n$ $0kl$: $l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
					Special: no extra conditions
2	*b*	2	$\frac{1}{2},\frac{1}{2},z$		
2	*a*	2	$0,0,z$		

*I*112

UNIQUE AXIS *c*, CELL CHOICE 3



Origin on 2

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

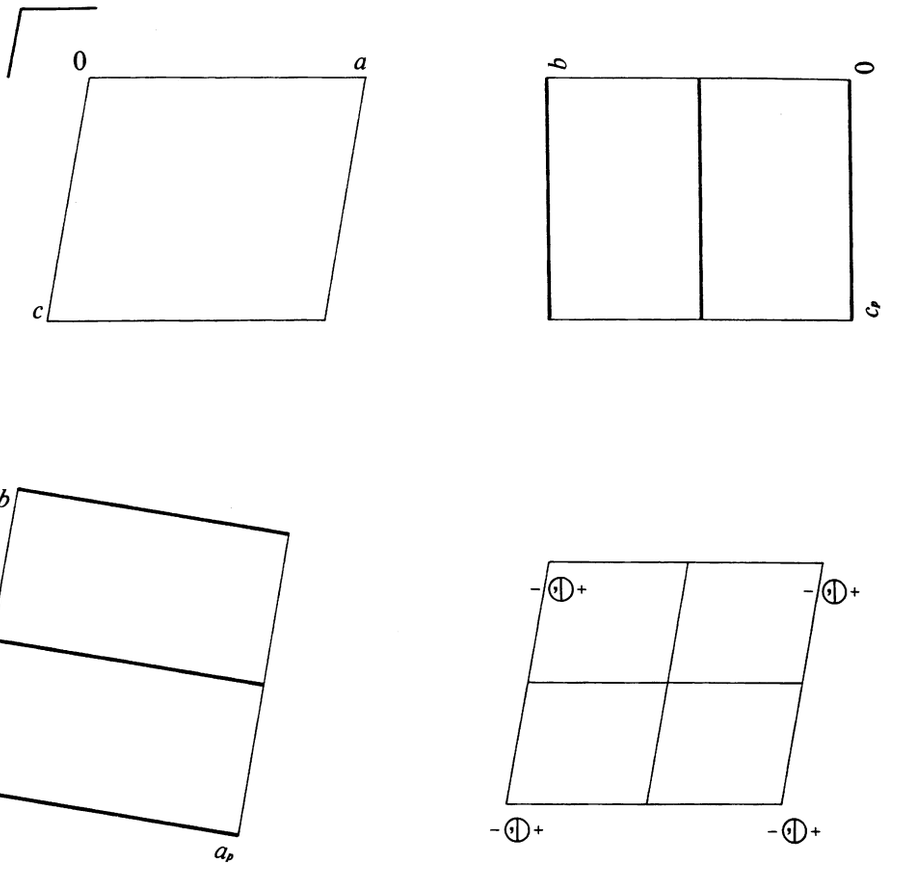
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	General:
4	*c*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
					Special: no extra conditions
2	*b*	2	$0,\frac{1}{2},z$		
2	*a*	2	$0,0,z$		

Pm C_s^1 m Monoclinic

No. 6 $P\,1\,m\,1$ Patterson symmetry $P\,1\,2/m\,1$

UNIQUE AXIS b



Origin on mirror plane m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) m $x,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $x,\bar{y},z$	no conditions
					Special: no extra conditions
1	b	m	$x,\frac{1}{2},z$		
1	a	m	$x,0,z$		

Symmetry of special projections

Along [001] $p\,1\,1\,m$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,1$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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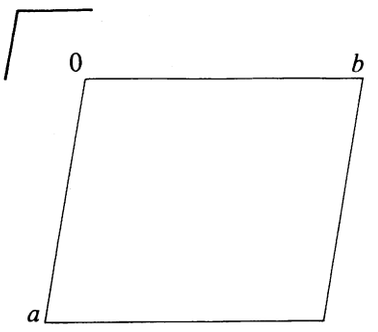
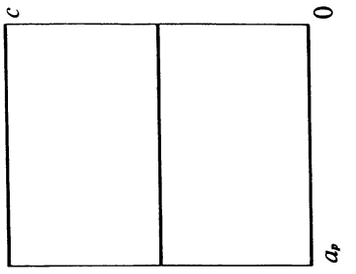
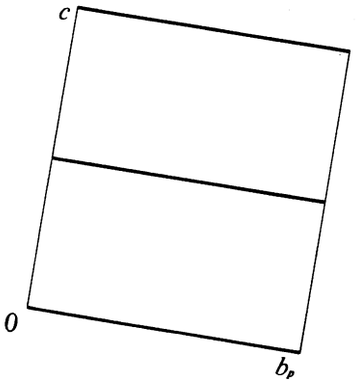
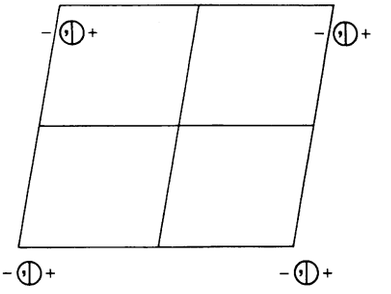








Origin on mirror plane m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) m $x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		Reflection conditions
					General:
2	c	1	(1) x,y,z	(2) $x,y,\bar{z}$	no conditions
					Special: no extra conditions
1	b	m	$x,y,\frac{1}{2}$		
1	a	m	$x,y,0$		

Symmetry of special projections

Along [001] $p\,1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

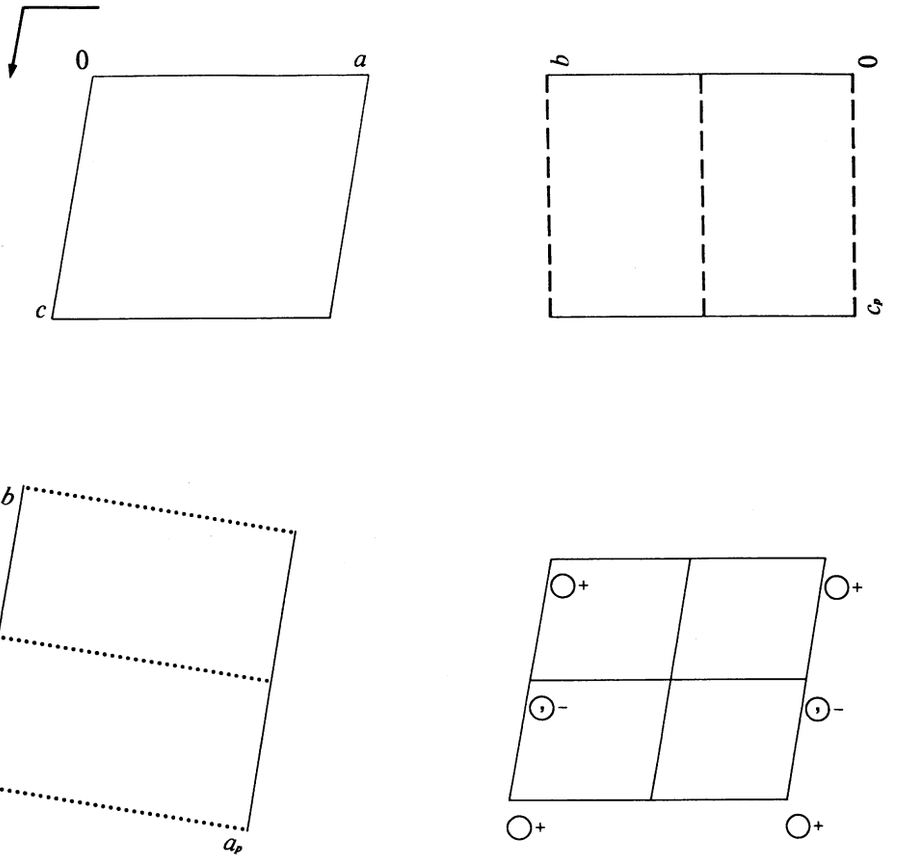
Along [100] $p\,1\,1\,m$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,m\,1$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

Pc C_s^2 m Monoclinic

No. 7 $P1c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) c $x,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x,\bar{y},z+\frac{1}{2}$	$h0l$: $l=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p\,1\,1\,m$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,g\,1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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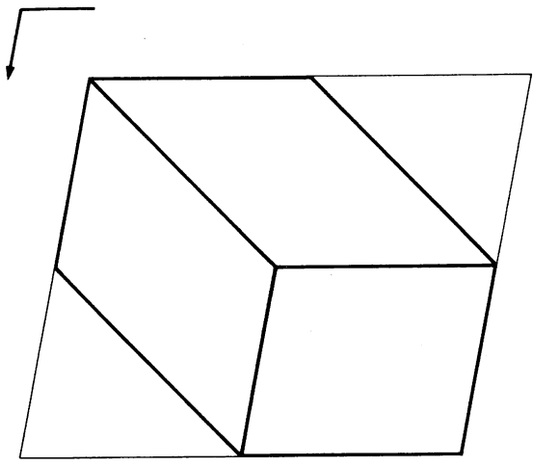
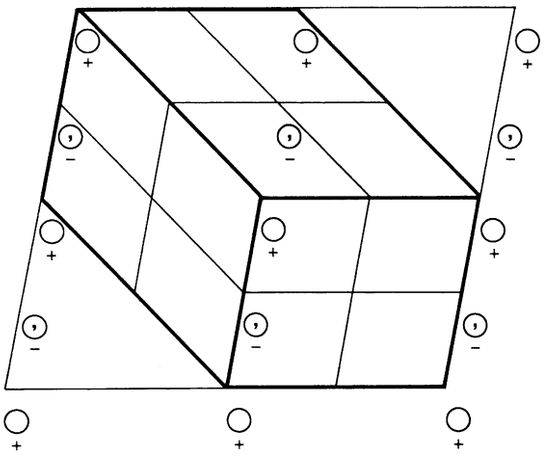
No. 7

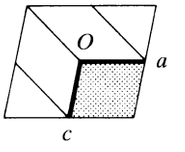
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P1c1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

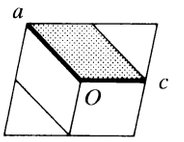
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x,\bar{y},z+\frac{1}{2}$	$h0l$: $l=2n$ $00l$: $l=2n$

P 1 *n* 1

UNIQUE AXIS *b*, CELL CHOICE 2



Origin on glide plane *n*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

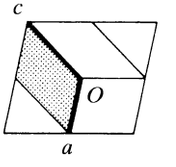
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	*a* 1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	$h0l$: $h+l=2n$ $h00$: $h=2n$ $00l$: $l=2n$

P 1 *a* 1

UNIQUE AXIS *b*, CELL CHOICE 3



Origin on glide plane *a*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

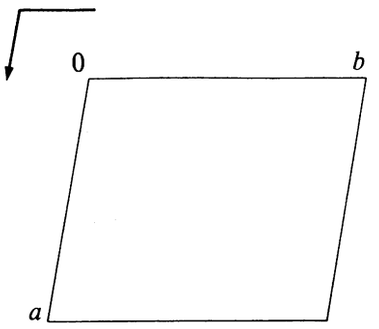
Positions

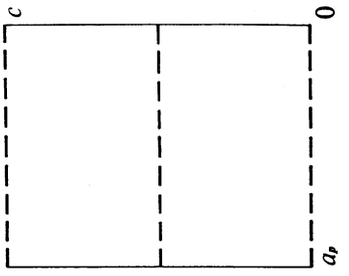
Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	*a* 1	(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z$	$h0l$: $h=2n$ $h00$: $h=2n$

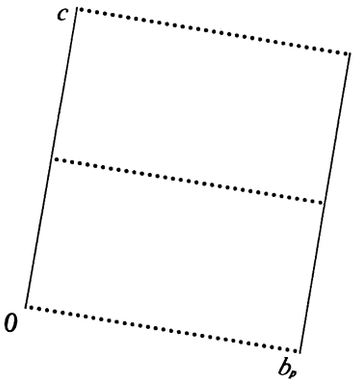
Monoclinic m C_s^2 Pc

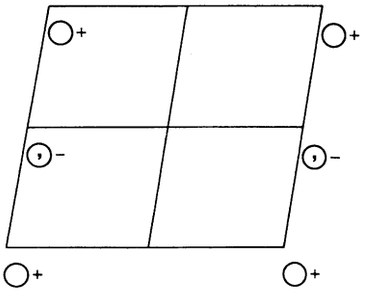
Patterson symmetry $P\,1\,1\,2/m$ $P\,1\,1\,a$ No. 7

UNIQUE AXIS c, CELL CHOICE 1









Origin on glide plane a

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) a $x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
			General:
2 a 1	(1) x,y,z	(2) $x+\frac{1}{2},y,\bar{z}$	$hk0$: $h=2n$ $h00$: $h=2n$

Symmetry of special projections

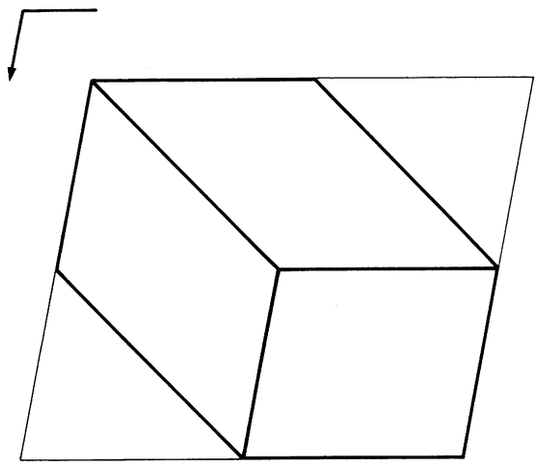
Along [001] $p\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

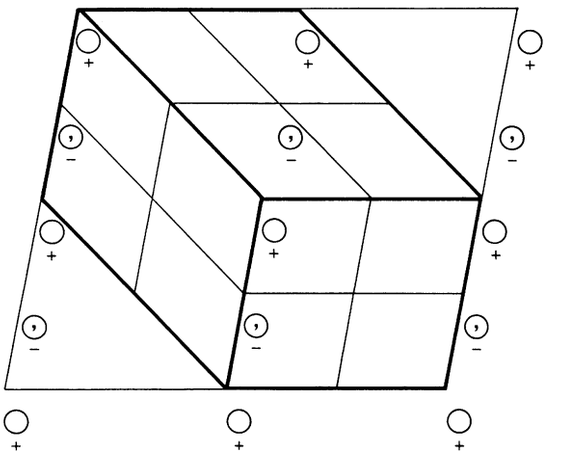
Along [100] $p\,1\,1\,m$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,g\,1$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

No. 7

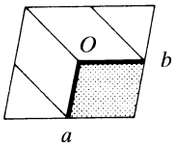
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$P\,1\,1\,a$

UNIQUE AXIS c, CELL CHOICE 1



Origin on glide plane a

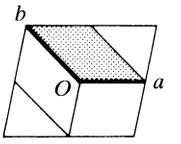
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	a	1	(1) x,y,z (2) $x+\frac{1}{2},y,\bar{z}$	$hk0$: $h=2n$ $h00$: $h=2n$

P 1 1 *n*



UNIQUE AXIS *c*, CELL CHOICE 2

Origin on glide plane *n*

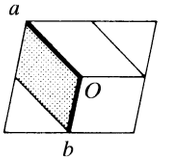
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	*a* 1	(1) x,y,z	(2) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	$hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$

P 1 1 *b*



UNIQUE AXIS *c*, CELL CHOICE 3

Origin on glide plane *b*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

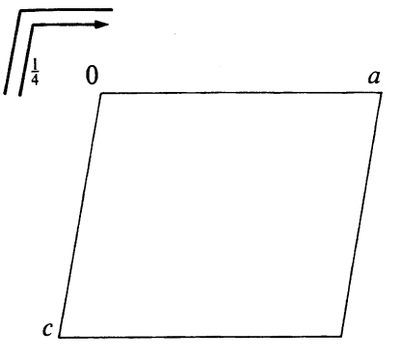
Positions

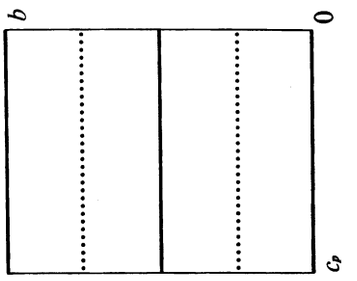
Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
2	*a* 1	(1) x,y,z	(2) $x,y+\frac{1}{2},\bar{z}$	$hk0$: $k=2n$ $0k0$: $k=2n$

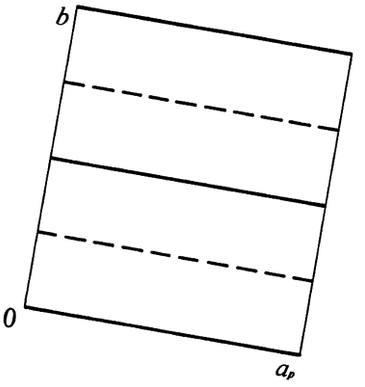
Cm C_s^3 m Monoclinic

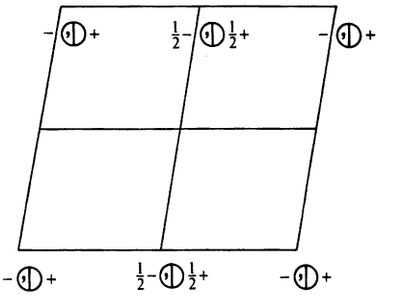
No. 8 $C\,1\,m\,1$ Patterson symmetry $C\,1\,2/m\,1$

UNIQUE AXIS b, CELL CHOICE 1









Origin on mirror plane m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) m $x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) a $x,\frac{1}{4},z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
				General:
4 *b* 1	(1) x,y,z	(2) $x,\bar{y},z$		hkl: $h+k=2n$ $h0l$: $h=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
				Special: no extra conditions
2 *a* *m*	$x,0,z$			

Symmetry of special projections

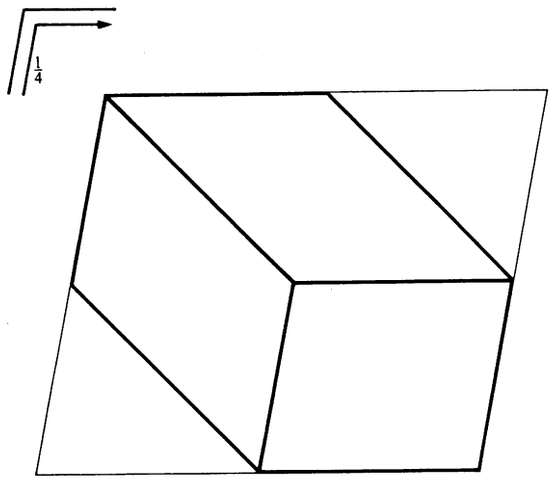
Along [001] $c\,1\,1\,m$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

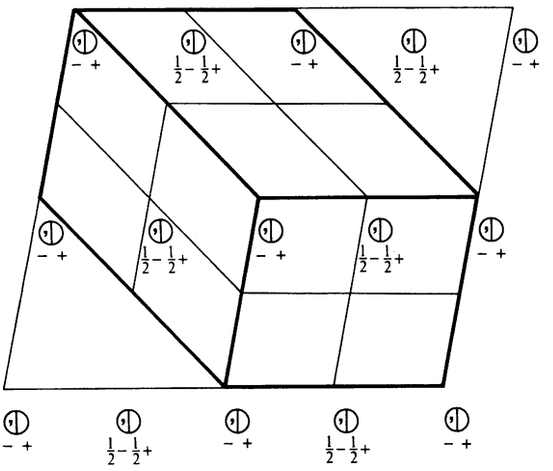
Along [100] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,1$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

No. 8

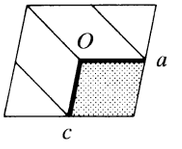
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C1m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on mirror plane m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

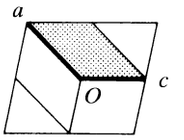
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
			General:
4 b 1	(1) x,y,z	(2) $x,\bar{y},z$	hkl: $h+k=2n$ $h0l$: $h=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
			Special: no extra conditions
2 a m	$x,0,z$		

A 1 *m* 1

UNIQUE AXIS *b*, CELL CHOICE 2



Origin on mirror plane *m*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$
4	*b*	1	(1) x,y,z	(2) $x,\bar{y},z$
2	*a*	*m*	$x,0,z$	

Reflection conditions

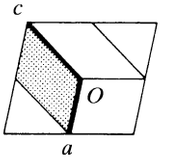
General:

hkl: $k+l=2n$
$h0l$: $l=2n$
$0kl$: $k+l=2n$
$hk0$: $k=2n$
$0k0$: $k=2n$
$00l$: $l=2n$

Special: no extra conditions

I 1 *m* 1

UNIQUE AXIS *b*, CELL CHOICE 3



Origin on mirror plane *m*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
4	*b*	1	(1) x,y,z	(2) $x,\bar{y},z$
2	*a*	*m*	$x,0,z$	

Reflection conditions

General:

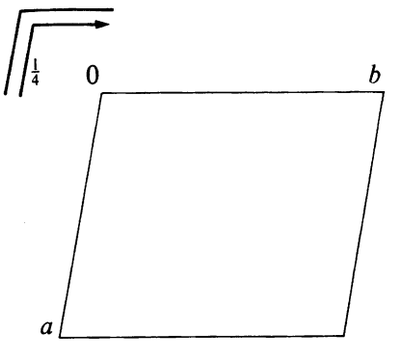
hkl: $h+k+l=2n$
$h0l$: $h+l=2n$
$0kl$: $k+l=2n$
$hk0$: $h+k=2n$
$0k0$: $k=2n$
$h00$: $h=2n$
$00l$: $l=2n$

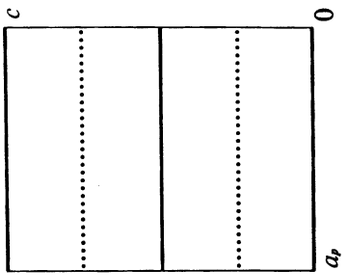
Special: no extra conditions

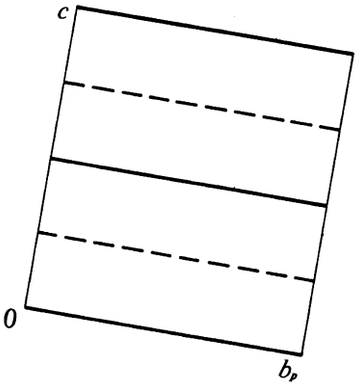
No. 8 $A\,1\,1\,m$

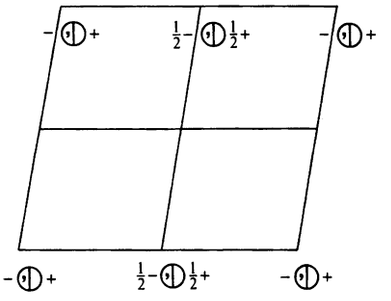
Patterson symmetry $A\,1\,1\,2/m$

UNIQUE AXIS c, CELL CHOICE 1









Origin on mirror plane m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) m $x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) b $x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$	Reflection conditions
			General:
4 *b* 1	(1) x,y,z	(2) $x,y,\bar{z}$	hkl: $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
			Special: no extra conditions
2 *a* *m*	$x,y,0$		

Symmetry of special projections

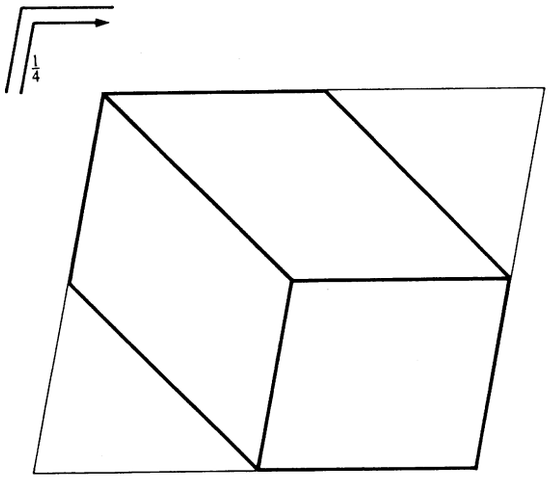
Along [001] $p\,1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

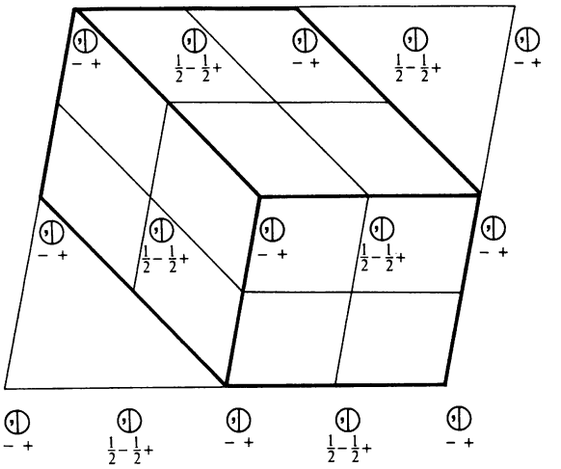
Along [100] $c\,1\,1\,m$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

No. 8

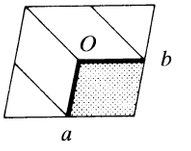
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A11m$

UNIQUE AXIS c, CELL CHOICE 1



Origin on mirror plane m

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

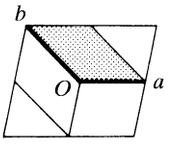
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4 b 1		(1) x,y,z	(2) $x,y,\bar{z}$	hkl: $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
2 a m		$x,y,0$		Special: no extra conditions

B 1 1 *m*

UNIQUE AXIS *c*, CELL CHOICE 2



Origin on mirror plane *m*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

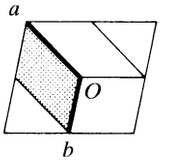
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		$(0,0,0)+$	$(\frac{1}{2},0,\frac{1}{2})+$	General:
4 *b* 1		(1) x,y,z	(2) $x,y,\bar{z}$	hkl: $h+l=2n$ $hk0$: $h=2n$ $0kl$: $l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
				Special: no extra conditions
2 *a* *m*		$x,y,0$		

I 1 1 *m*

UNIQUE AXIS *c*, CELL CHOICE 3



Origin on mirror plane *m*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

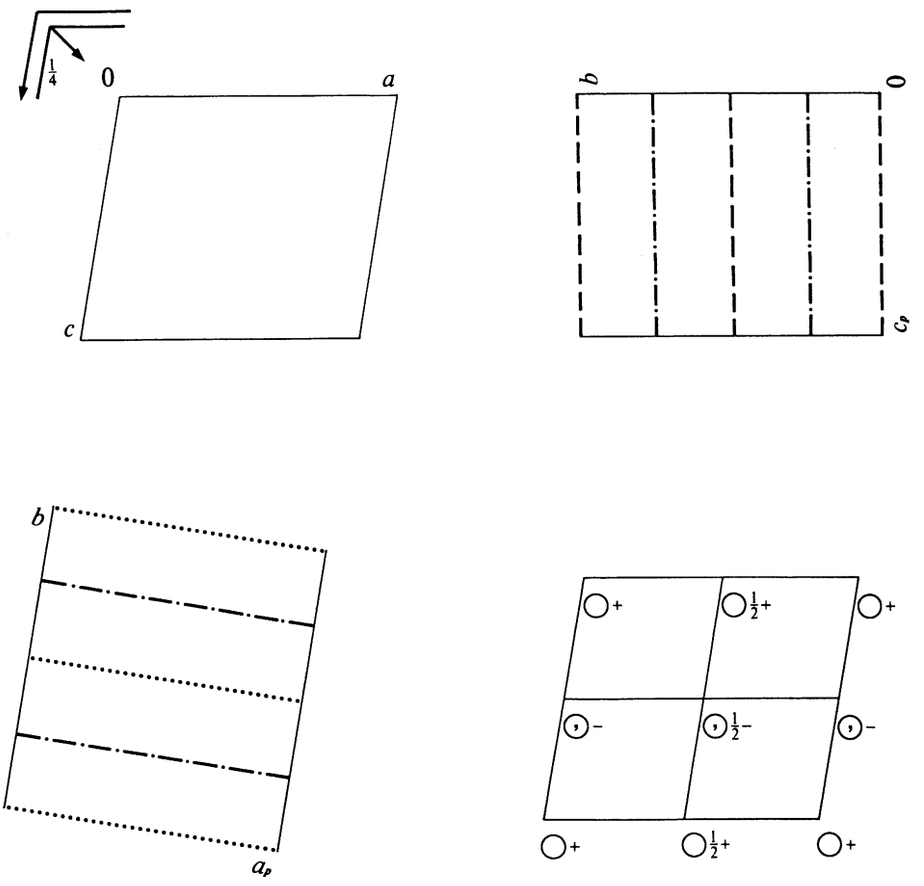
Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	General:
4 *b* 1		(1) x,y,z	(2) $x,y,\bar{z}$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
				Special: no extra conditions
2 *a* *m*		$x,y,0$		

Cc C_s^4 m Monoclinic

No. 9 $C1c1$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) c $x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$	Coordinates $(\frac{1}{2},\frac{1}{2},0)+$
4 a 1		(1) x,y,z	(2) $x,\bar{y},z+\frac{1}{2}$

Reflection conditions

General:

hkl: $h+k=2n$
$h0l$: $h,l=2n$
$0kl$: $k=2n$
$hk0$: $h+k=2n$
$0k0$: $k=2n$
$h00$: $h=2n$
$00l$: $l=2n$

Symmetry of special projections

Along [001] $c1\,1\,m$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

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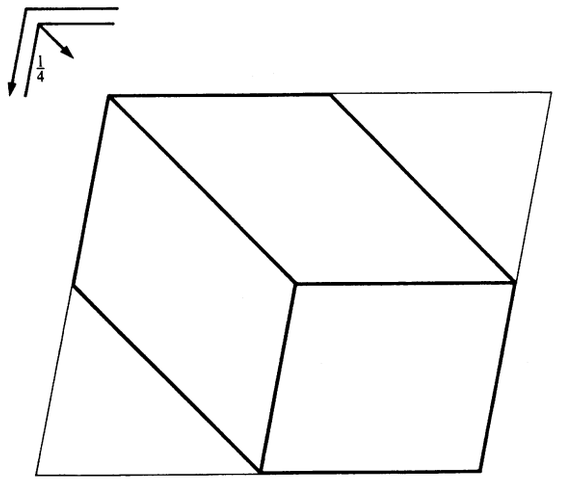
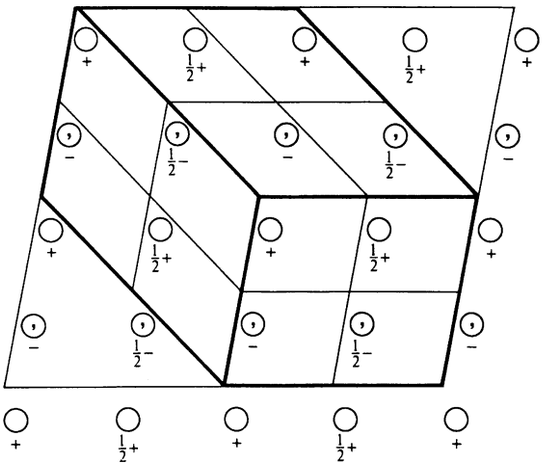
No. 9

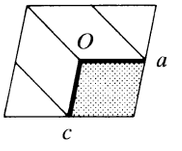
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C1c1$

UNIQUE AXIS b, CELL CHOICE 1



Origin on glide plane c

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates (0,0,0)+	Coordinates $(\frac{1}{2},\frac{1}{2},0)+$
4 a 1		(1) x,y,z	(2) $x,\bar{y},z+\frac{1}{2}$

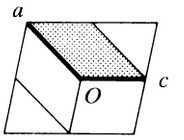
Reflection conditions

General:

hkl: $h+k=2n$
$h0l$: $h,l=2n$
$0kl$: $k=2n$
$hk0$: $h+k=2n$
$0k0$: $k=2n$
$h00$: $h=2n$
$00l$: $l=2n$

A 1 *n* 1

UNIQUE AXIS *b*, CELL CHOICE 2



Origin on glide plane *n*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

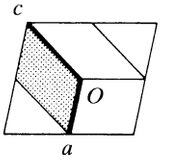
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4 *a* 1		(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	hkl: $k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$

I 1 *a* 1

UNIQUE AXIS *b*, CELL CHOICE 3



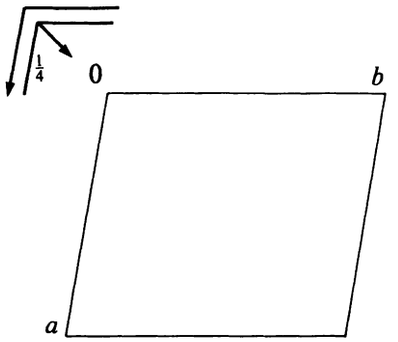
Origin on glide plane *a*

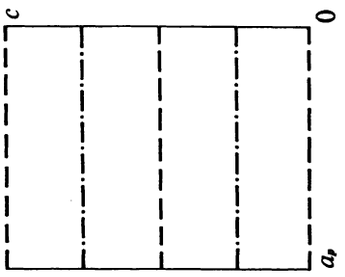
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

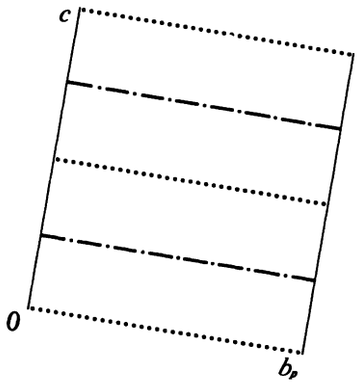
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

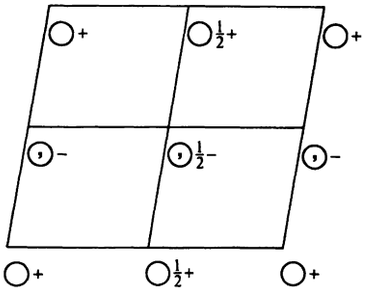
Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
		$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	General:
4 *a* 1		(1) x,y,z	(2) $x+\frac{1}{2},\bar{y},z$	hkl: $h+k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$









Origin on glide plane a

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) a $x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates		Reflection conditions
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	General:
4 a 1	(1) x,y,z	(2) $x+\frac{1}{2},y,\bar{z}$	hkl: $k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$

Symmetry of special projections

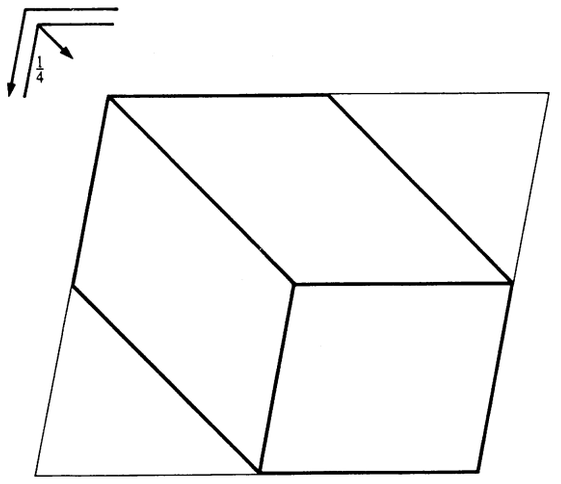
Along [001] $p\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

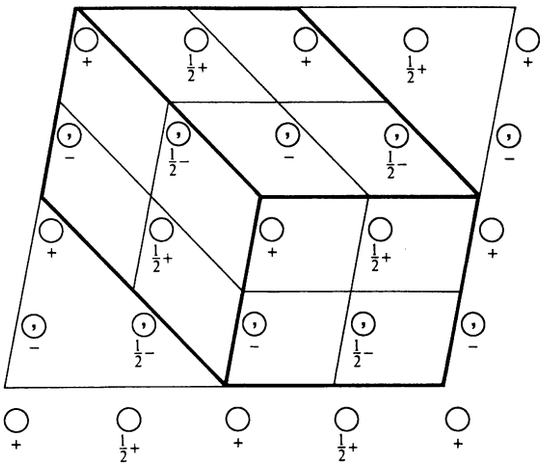
Along [100] $c\,1\,1\,m$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,g\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

No. 9

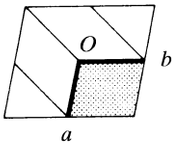
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A11a$

UNIQUE AXIS c, CELL CHOICE 1



Origin on glide plane a

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

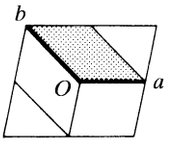
Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$	
4 a 1	(1) x,y,z	(2) $x+\frac{1}{2},y,\bar{z}$	

Reflection conditions

General:

hkl: $k+l=2n$
$hk0$: $h,k=2n$
$0kl$: $k+l=2n$
$h0l$: $l=2n$
$00l$: $l=2n$
$h00$: $h=2n$
$0k0$: $k=2n$

B 1 1 *n*



UNIQUE AXIS *c*, CELL CHOICE 2

Origin on glide plane *n*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2)

Positions

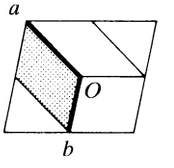
Multiplicity, Wyckoff letter, Site symmetry		Coordinates	
		$(0,0,0)+$	$(\frac{1}{2},0,\frac{1}{2})+$
4 *a* 1		(1) x,y,z	(2) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$

Reflection conditions

General:

hkl: $h+l=2n$
$hk0$: $h,k=2n$
$0kl$: $l=2n$
$h0l$: $h+l=2n$
$00l$: $l=2n$
$h00$: $h=2n$
$0k0$: $k=2n$

I 1 1 *b*



UNIQUE AXIS *c*, CELL CHOICE 3

Origin on glide plane *b*

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates	
		$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$
4 *a* 1		(1) x,y,z	(2) $x,y+\frac{1}{2},\bar{z}$

Reflection conditions

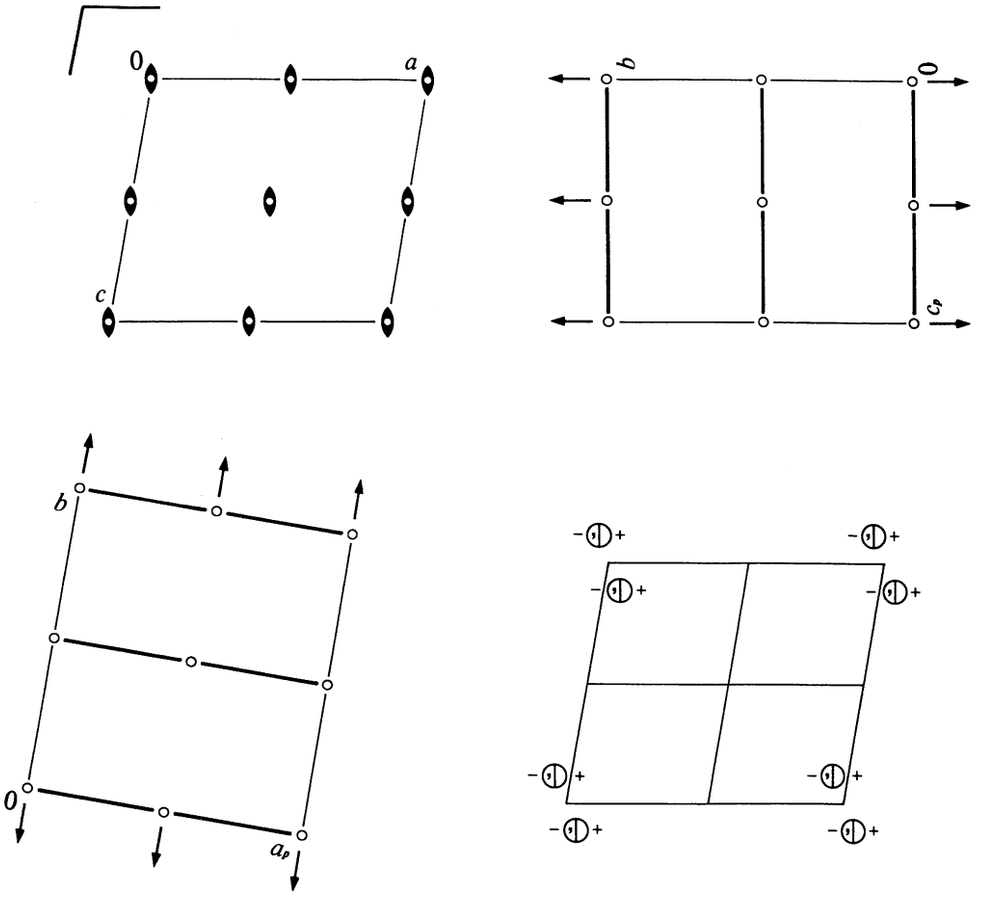
General:

hkl: $h+k+l=2n$
$hk0$: $h,k=2n$
$0kl$: $k+l=2n$
$h0l$: $h+l=2n$
$00l$: $l=2n$
$h00$: $h=2n$
$0k0$: $k=2n$

$P2/m$ C_{2h}^1 $2/m$ Monoclinic

No. 10 $P12/m1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,y,0$ (3) $\bar{1}$ $0,0,0$ (4) m $x,0,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	o	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	no conditions
							Special: no extra conditions
2	n	m	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$			
2	m	m	$x,0,z$	$\bar{x},0,\bar{z}$			
2	l	2	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$			
2	k	2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	j	2	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	i	2	$0,y,0$	$0,\bar{y},0$			
1	h	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				
1	f	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				
1	e	$2/m$	$\frac{1}{2},\frac{1}{2},0$				
1	d	$2/m$	$\frac{1}{2},0,0$				
1	c	$2/m$	$0,0,\frac{1}{2}$				
1	b	$2/m$	$0,\frac{1}{2},0$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

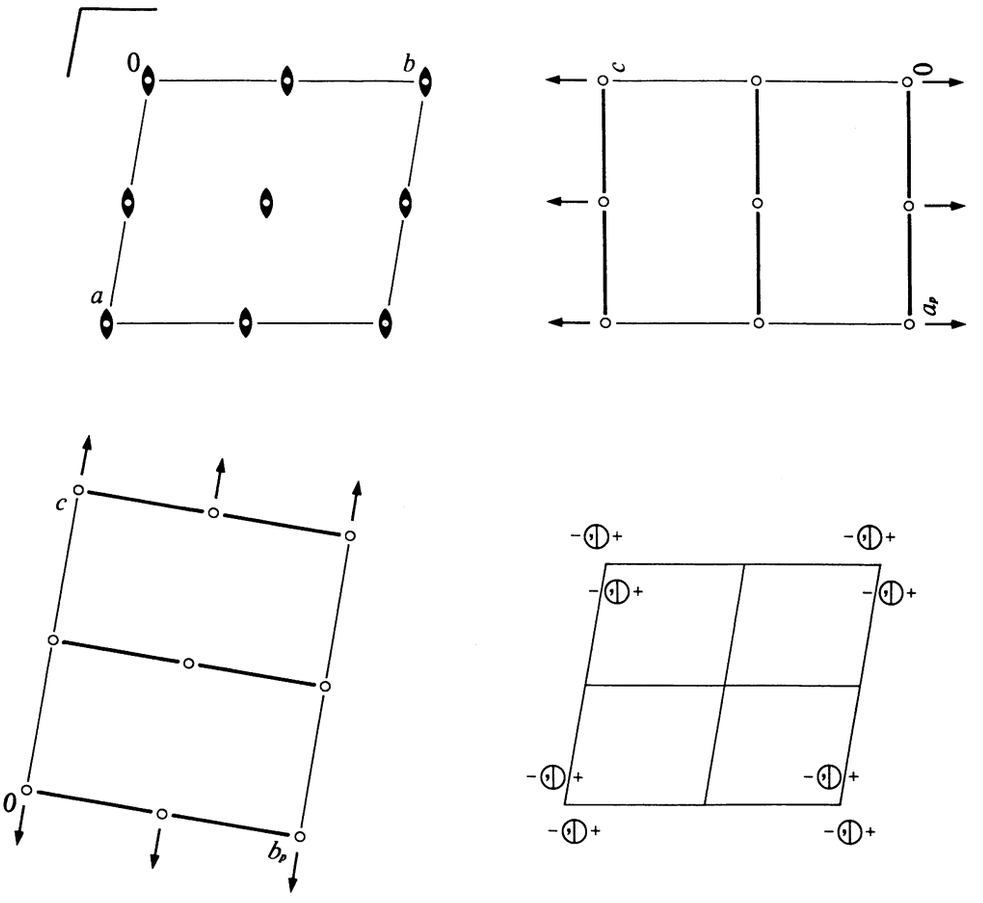
Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

No. 10 $P112/m$

Patterson symmetry $P112/m$

UNIQUE AXIS c



Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{1}$ $0,0,0$ (4) m $x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	o	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	no conditions
							Special: no extra conditions
2	n	m	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$			
2	m	m	$x,y,0$	$\bar{x},\bar{y},0$			
2	l	2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	k	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	j	2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	i	2	$0,0,z$	$0,0,\bar{z}$			
1	h	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	$2/m$	$\frac{1}{2},\frac{1}{2},0$				
1	f	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				
1	e	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				
1	d	$2/m$	$0,\frac{1}{2},0$				
1	c	$2/m$	$\frac{1}{2},0,0$				
1	b	$2/m$	$0,0,\frac{1}{2}$				
1	a	$2/m$	$0,0,0$				

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

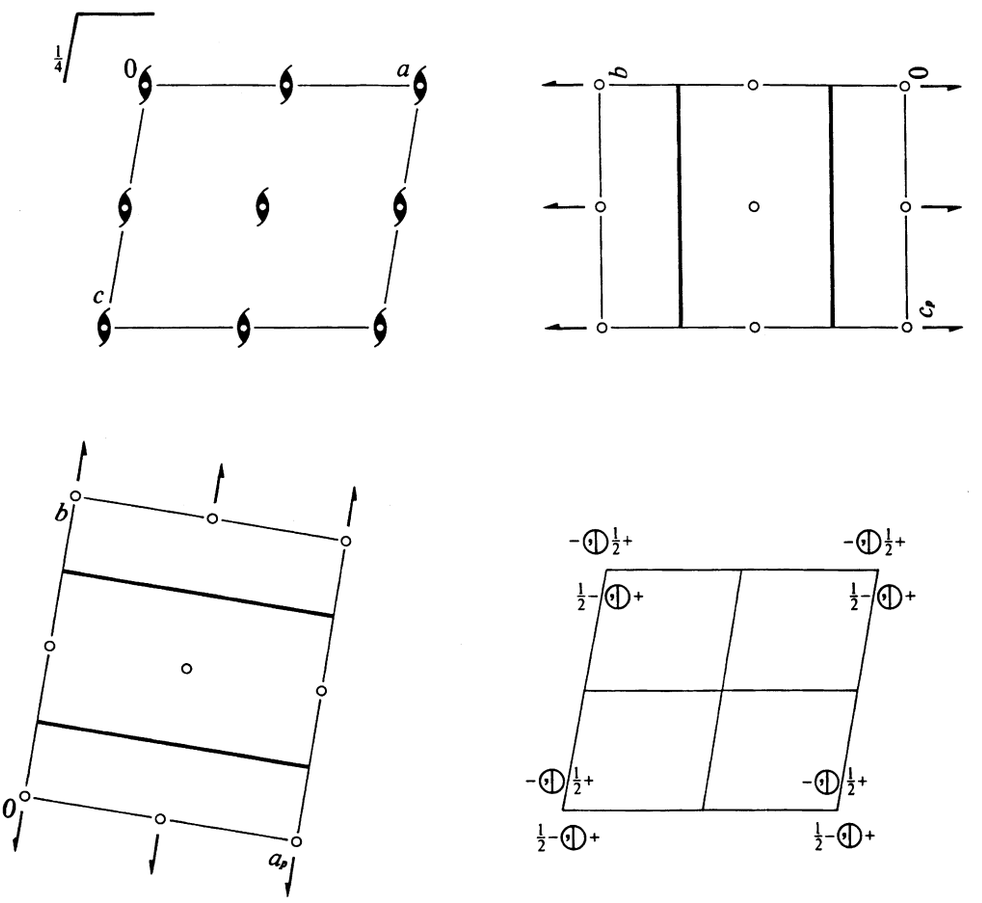
Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

$P2_1/m$ C_{2h}^2 $2/m$ Monoclinic

No. 11 $P12_1/m1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b



Origin at $\bar{1}$ on 2_1

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,0$ (3) $\bar{1}$ $0,0,0$ (4) m $x,\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z$	$0k0$: $k=2n$
							Special: as above, plus
2	e	m	$x,\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $k=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$			hkl: $k=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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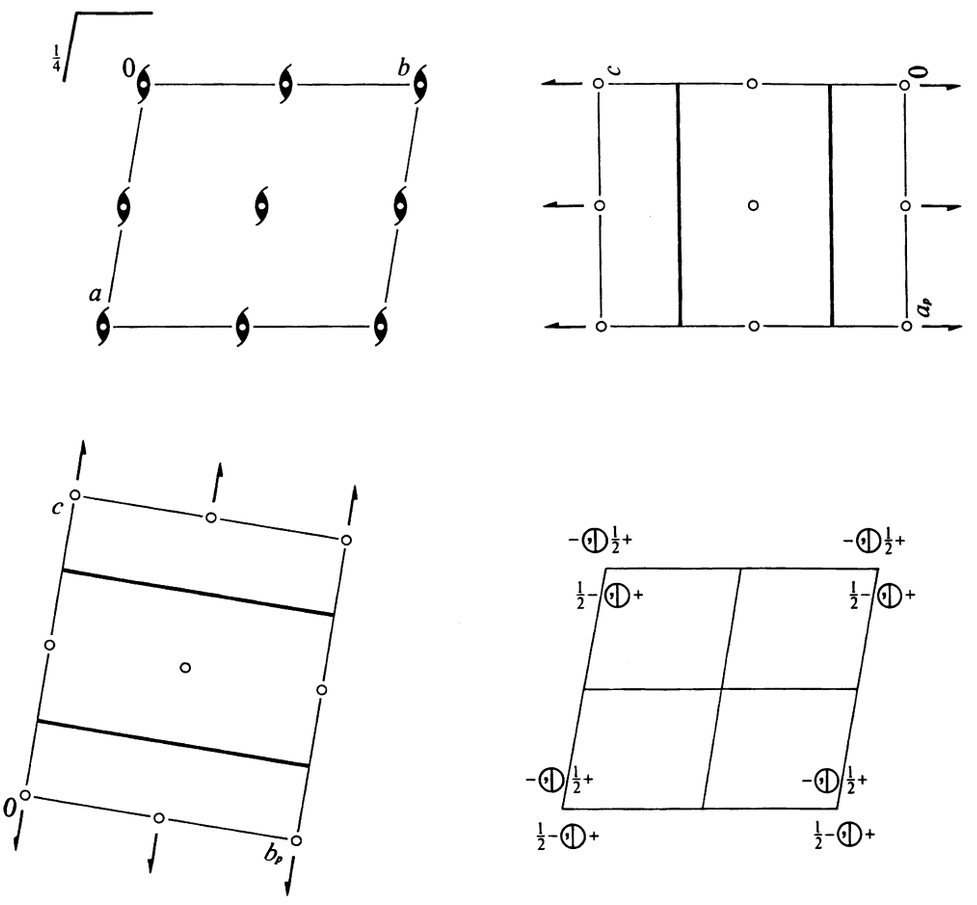


Origin at $\bar{1}$ on 2_1

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $\bar{1}$ $0,0,0$ (4) m $x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
2	e	m	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

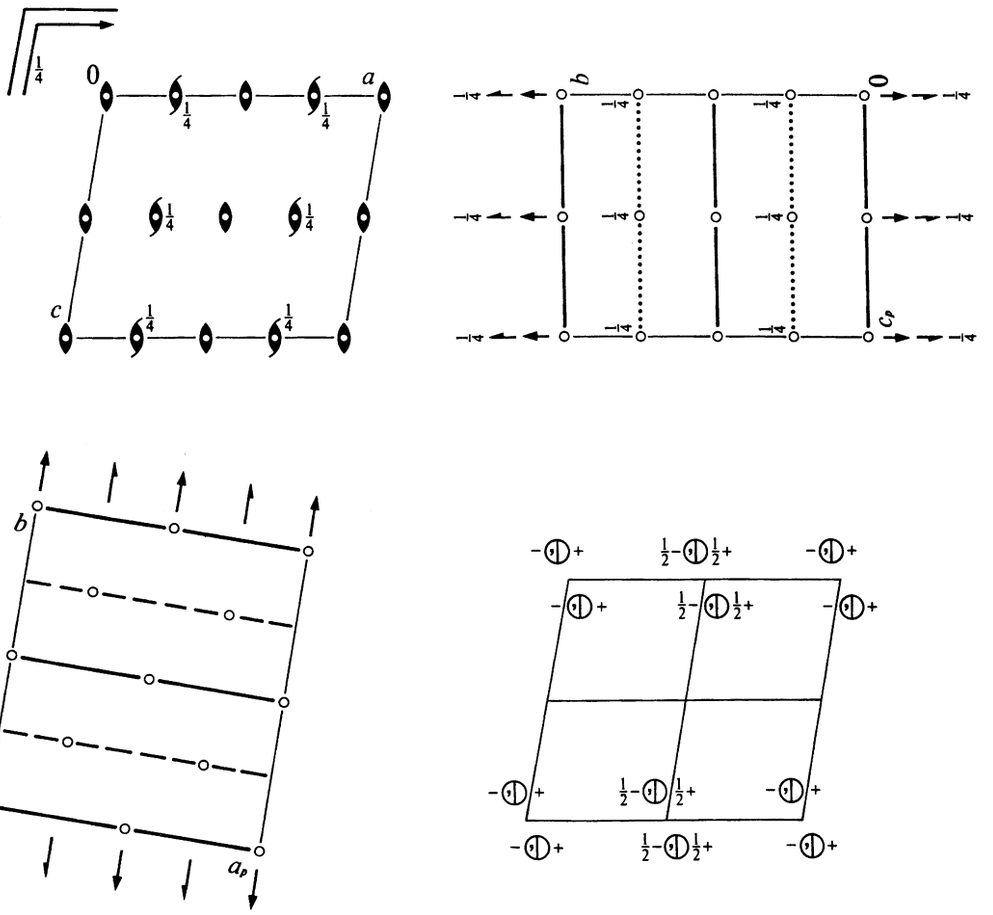
Along [100] $p2gm$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

$C2/m$ C_{2h}^3 $2/m$ Monoclinic

No. 12 $C12/m1$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,y,0$ (3) $\bar{1}$ $0,0,0$ (4) m $x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (3) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ (4) a $x,\frac{1}{4},z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	hkl: $h+k=2n$ $h0l$: $h=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$			no extra conditions
4	h	2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	g	2	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $h=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl: $h=2n$
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2	c	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

Symmetry of special projections

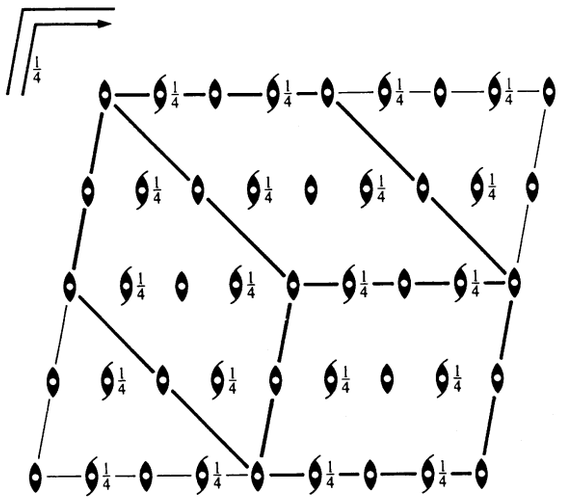
Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

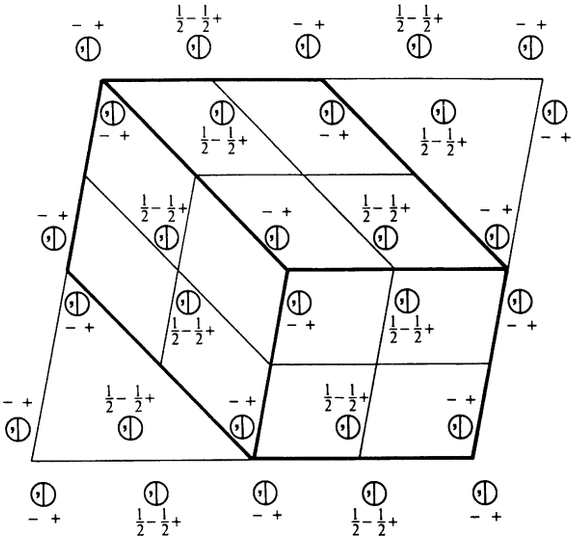
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

No. 12

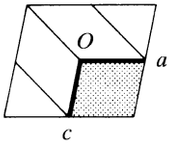
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at centre $(2/m)$

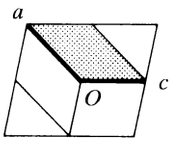
Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			
8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	General:
							hkl: $h+k=2n$ $hk0$: $h+k=2n$
							$h0l$: $h=2n$ $0k0$: $k=2n$
							$0kl$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$			no extra conditions
4	h	2	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	g	2	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $h=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2	c	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

$A12/m1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at centre $(2/m)$

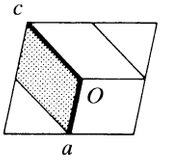
Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (0,\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	hkl: $k+l=2n$ $\quad$ $hk0$: $k=2n$ $h0l$: $l=2n$ $\quad$ $0kl$: $k=2n$ $0kl$: $k+l=2n$ $\quad$ $00l$: $l=2n$
							Special: as above, plus
4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$			no extra conditions
4	h	2	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$			no extra conditions
4	g	2	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$			hkl: $k=2n$
4	e	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$			
2	d	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
2	c	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

$I12/m1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

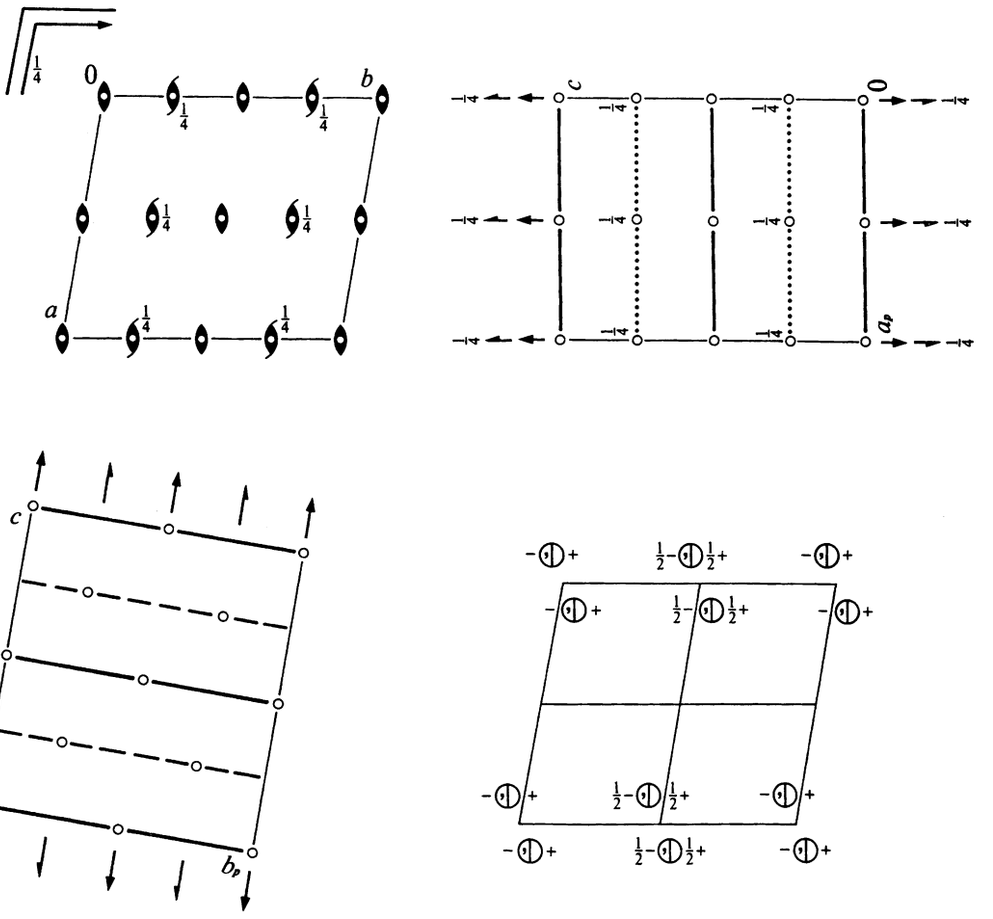
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	j	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z$	hkl: $h+k+l=2n$ $\quad$ $0k0$: $k=2n$ $h0l$: $h+l=2n$ $\quad$ $h00$: $h=2n$ $0kl$: $k+l=2n$ $\quad$ $00l$: $l=2n$ $hk0$: $h+k=2n$
							Special: as above, plus
4	i	m	$x,0,z$	$\bar{x},0,\bar{z}$			no extra conditions
4	h	2	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			no extra conditions
4	g	2	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl: $k=2n$
4	e	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			
2	d	$2/m$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	c	$2/m$	$\frac{1}{2},0,0$				no extra conditions
2	b	$2/m$	$0,\frac{1}{2},0$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

No. 12 $A112/m$

Patterson symmetry $A112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) $\bar{1}$ $0,0,0$ (4) m $x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$ (4) b $x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$			General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	hkl: $k+l=2n$ $hk0$: $k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	i	m	$x,y,0$	$\bar{x},\bar{y},0$			no extra conditions
4	h	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
4	g	2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			hkl: $k=2n$
4	e	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl: $k=2n$
2	d	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	c	$2/m$	$\frac{1}{2},0,0$				no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

Symmetry of special projections

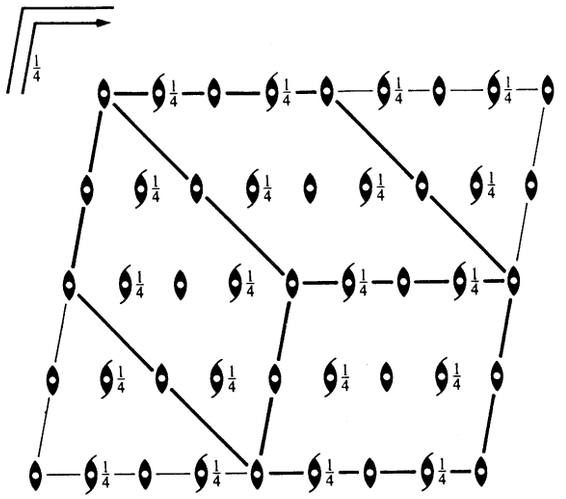
Along [001] $p2$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

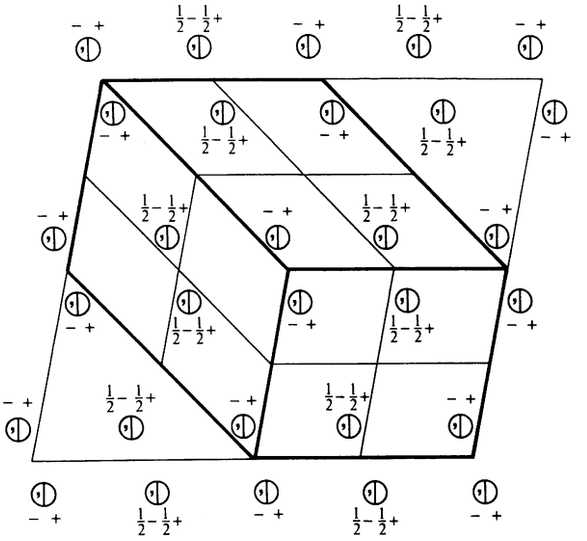
Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

No. 12

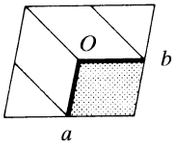
UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at centre $(2/m)$

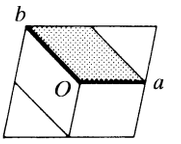
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$			General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	hkl: $k+l=2n$ $\quad h0l$: $l=2n$ $hk0$: $k=2n$ $\quad 00l$: $l=2n$ $0kl$: $k+l=2n$ $\quad 0k0$: $k=2n$
							Special: as above, plus
4	i	m	$x,y,0$	$\bar{x},\bar{y},0$			no extra conditions
4	h	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
4	g	2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	f	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			hkl: $k=2n$
4	e	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			
2	d	$2/m$	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	c	$2/m$	$\frac{1}{2},0,0$				no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

$B112/m$



UNIQUE AXIS c, CELL CHOICE 2

Origin at centre $(2/m)$

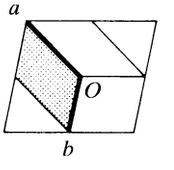
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},0,\frac{1}{2})+$				Reflection conditions
							General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	hkl: $h+l=2n$ $\quad$ $h0l$: $h+l=2n$ $hk0$: $h=2n$ $\quad$ $00l$: $l=2n$ $0kl$: $l=2n$ $\quad$ $h00$: $h=2n$
							Special: as above, plus
4	i	m	$x,y,0$	$\bar{x},\bar{y},0$			no extra conditions
4	h	2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
4	g	2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	f	$\bar{1}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$			hkl: $h=2n$
4	e	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$			
2	d	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
2	c	$2/m$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

$I112/m$



UNIQUE AXIS c, CELL CHOICE 3

Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

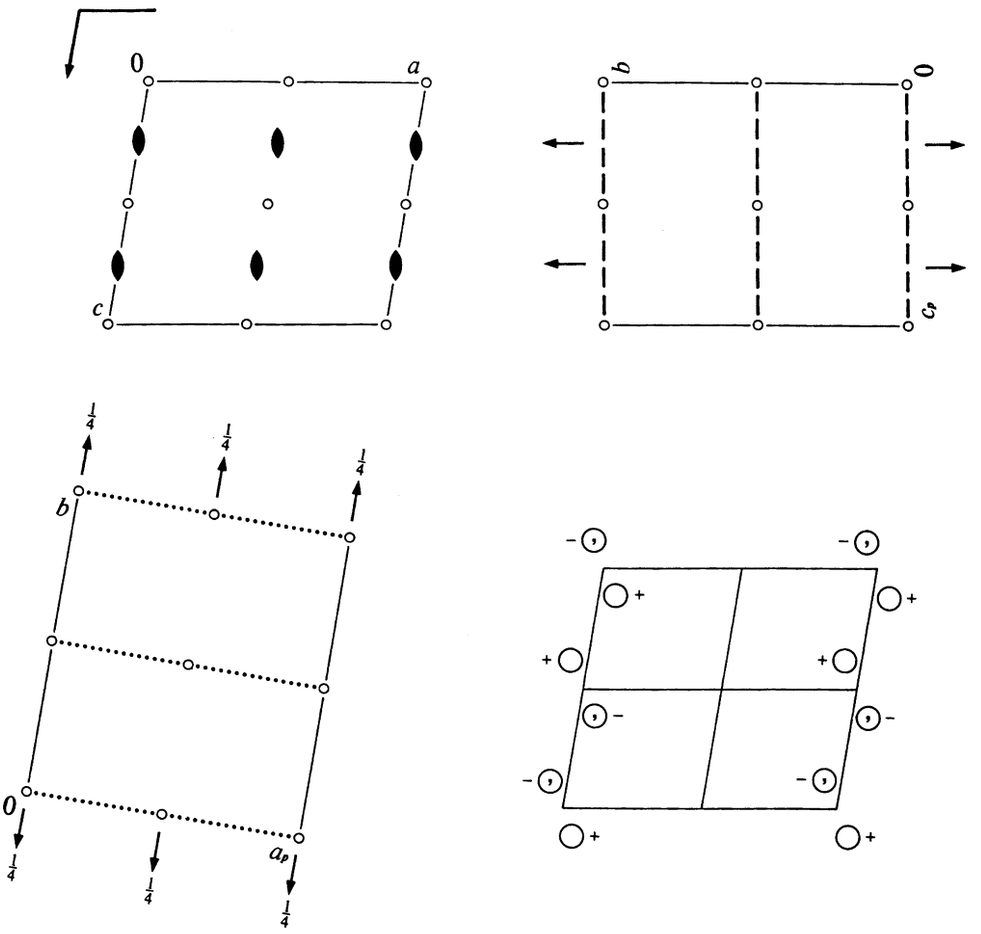
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$	hkl: $h+k+l=2n$ $\quad$ $00l$: $l=2n$ $hk0$: $h+k=2n$ $\quad$ $h00$: $h=2n$ $0kl$: $k+l=2n$ $\quad$ $0k0$: $k=2n$ $h0l$: $h+l=2n$
							Special: as above, plus
4	i	m	$x,y,0$	$\bar{x},\bar{y},0$			no extra conditions
4	h	2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	g	2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	f	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$			hkl: $l=2n$
4	e	$\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			
2	d	$2/m$	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2	c	$2/m$	$0,\frac{1}{2},0$				no extra conditions
2	b	$2/m$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$2/m$	$0,0,0$				no extra conditions

$P2/c$ C_{2h}^4 $2/m$ Monoclinic

No. 13 $P12/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane c

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,0,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	$h0l$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
2	f	2	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$			no extra conditions
2	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

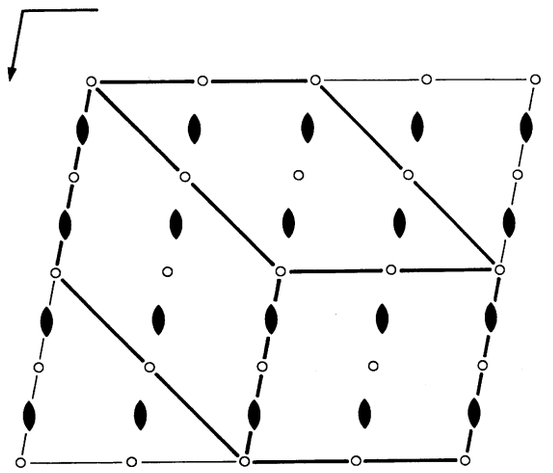
Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

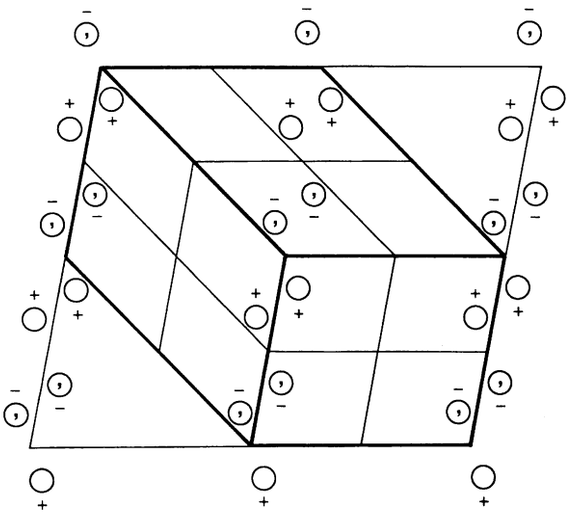
Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

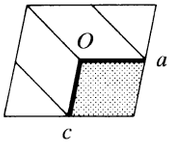
No. 13

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P12/c1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at $\bar{1}$ on glide plane c

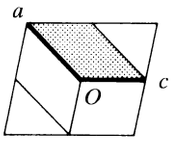
Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 g 1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	$h0l$: $l=2n$ $00l$: $l=2n$
					Special: as above, plus
2 f 2	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$			no extra conditions
2 e 2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
2 d $\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$	2 c $\bar{1}$	$0,\frac{1}{2},0$ $0,\frac{1}{2},\frac{1}{2}$	hkl: $l=2n$
2 b $\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	2 a $\bar{1}$	$0,0,0$ $0,0,\frac{1}{2}$	hkl: $l=2n$

$P12/n1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

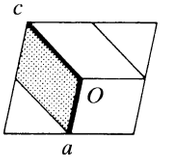
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$					$h0l$: $h+l=2n$ $h00$: $h=2n$ $00l$: $l=2n$
											Special: as above, plus
2	f	2	$\frac{3}{4},y,\frac{1}{4}$	$\frac{1}{4},\bar{y},\frac{3}{4}$							no extra conditions
2	e	2	$\frac{3}{4},y,\frac{3}{4}$	$\frac{1}{4},\bar{y},\frac{1}{4}$							no extra conditions
2	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$			2	c	$\bar{1}$	$0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			2	a	$\bar{1}$	$0,0,0$ $\frac{1}{2},0,\frac{1}{2}$	hkl: $h+l=2n$

$P12/a1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

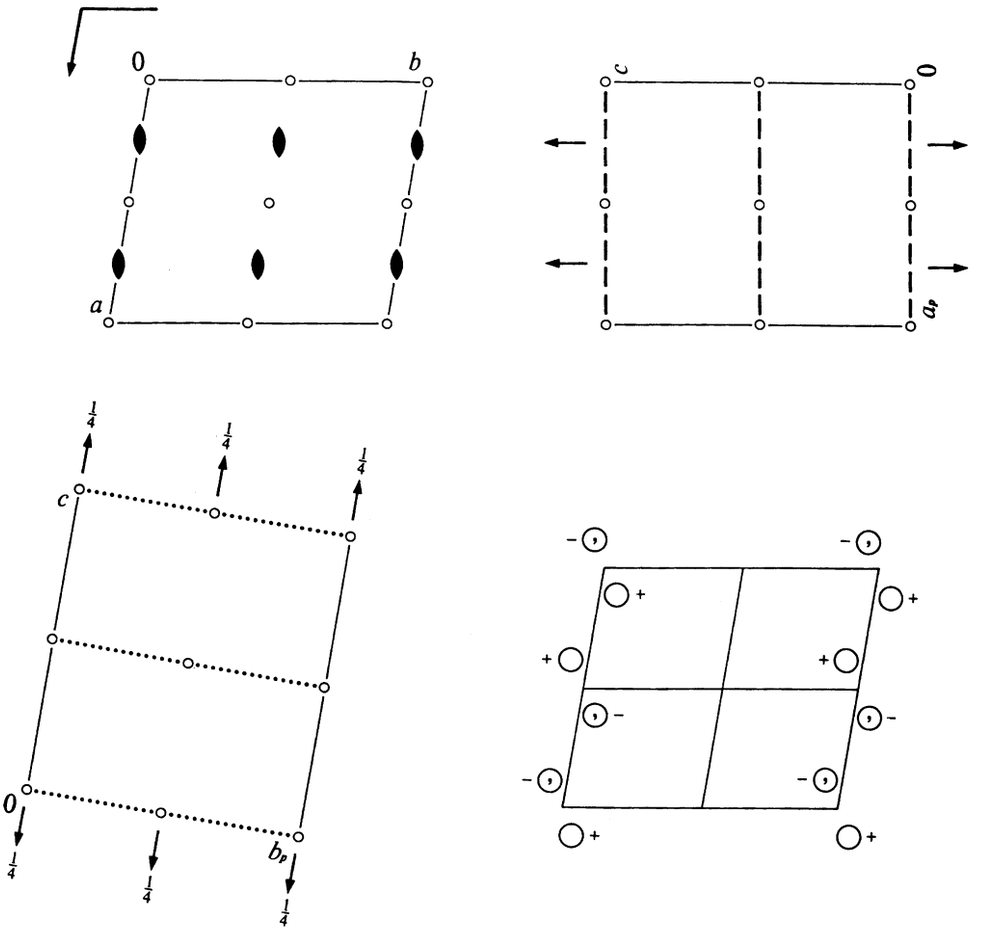
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z$					$h0l$: $h=2n$ $h00$: $h=2n$
											Special: as above, plus
2	f	2	$\frac{3}{4},y,\frac{1}{2}$	$\frac{1}{4},\bar{y},\frac{1}{2}$							no extra conditions
2	e	2	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y},0$							no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,0,\frac{1}{2}$			2	c	$\bar{1}$	$0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},0$	hkl: $h=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			2	a	$\bar{1}$	$0,0,0$ $\frac{1}{2},0,0$	hkl: $h=2n$

No. 13 $P112/a$

Patterson symmetry $P112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $\frac{1}{4},0,z$ (3) $\bar{1}$ $0,0,0$ (4) a $x,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	$hk0$: $h=2n$ $h00$: $h=2n$
							Special: as above, plus
2	f	2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			no extra conditions
2	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
2	d	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			hkl: $h=2n$

Symmetry of special projections

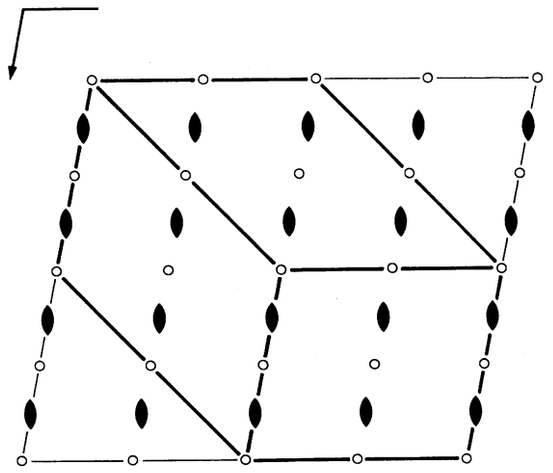
Along [001] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

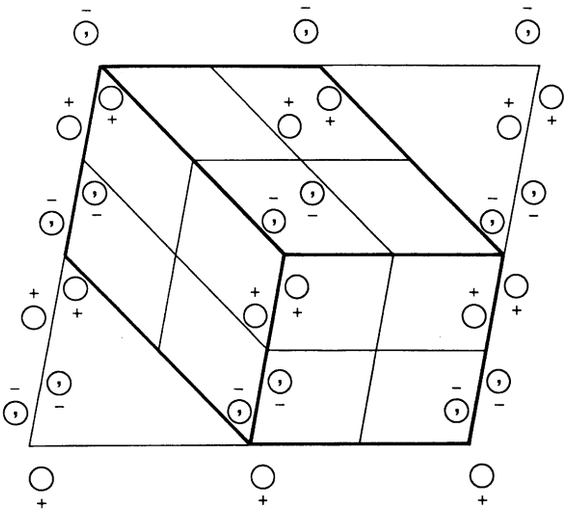
Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

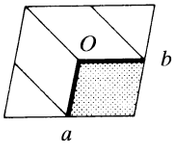
No. 13

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$P112/a$



UNIQUE AXIS c, CELL CHOICE 1

Origin at $\bar{1}$ on glide plane a

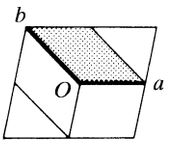
Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates							Reflection conditions
										General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$				$hk0$: $h=2n$ $h00$: $h=2n$
										Special: as above, plus
2	f	2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$						no extra conditions
2	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$						no extra conditions
2	d	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			2 c	$\bar{1}$	$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$	hkl: $h=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			2 a	$\bar{1}$	$0,0,0$ $\frac{1}{2},0,0$	hkl: $h=2n$

$P112/n$



UNIQUE AXIS c, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

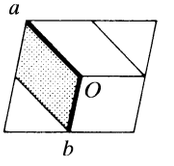
Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates							Reflection conditions
										General:
4	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$				$hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
										Special: as above, plus
2	f	2	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$						no extra conditions
2	e	2	$\frac{3}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$						no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+k=2n$

$P112/b$



UNIQUE AXIS c, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane b

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

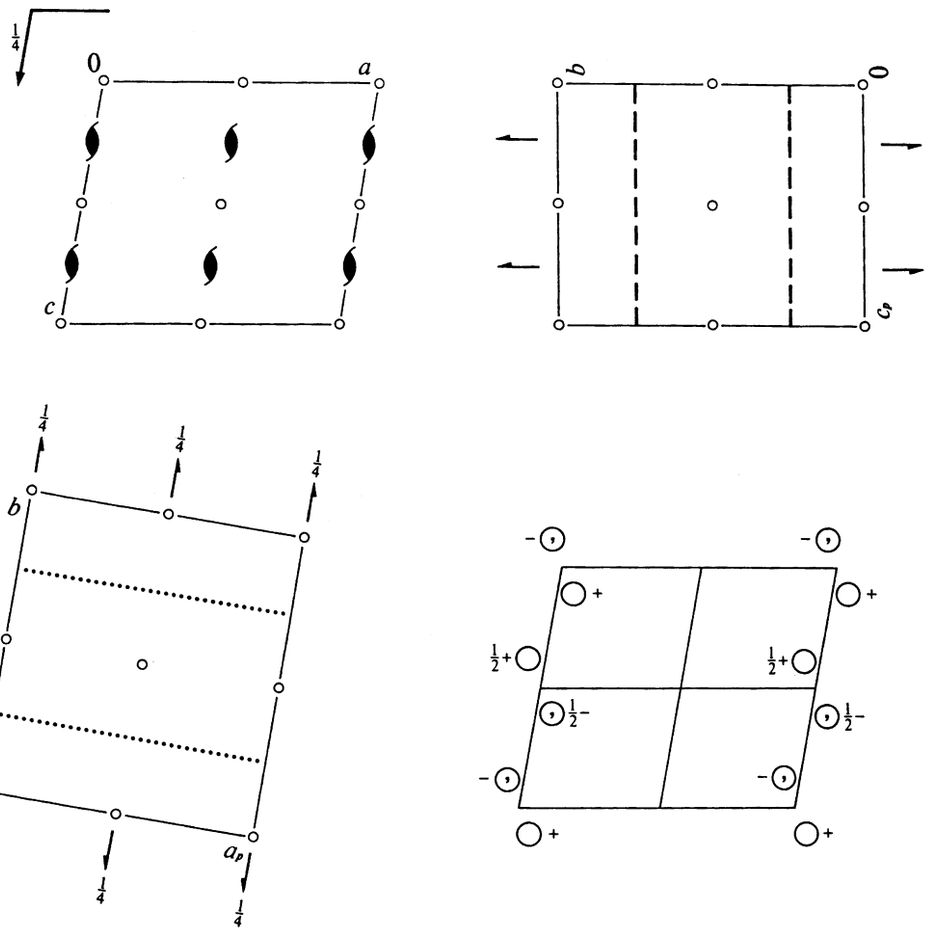
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates							Reflection conditions
										General:
4	g	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}$				$hk0$: $k=2n$ $0k0$: $k=2n$
										Special: as above, plus
2	f	2	$\frac{1}{2},\frac{3}{4},z$	$\frac{1}{2},\frac{1}{4},\bar{z}$						no extra conditions
2	e	2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$						no extra conditions
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $k=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$	hkl: $k=2n$

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

Symmetry of special projections

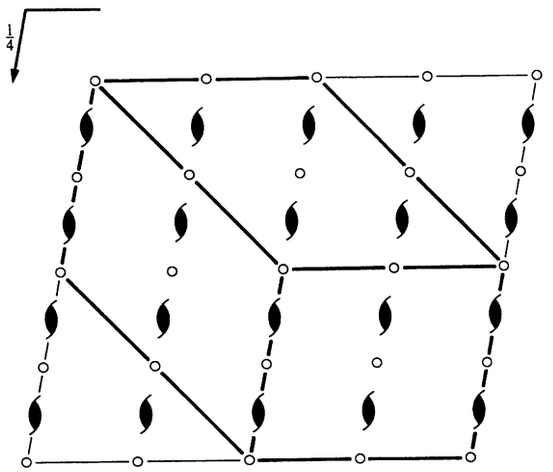
Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

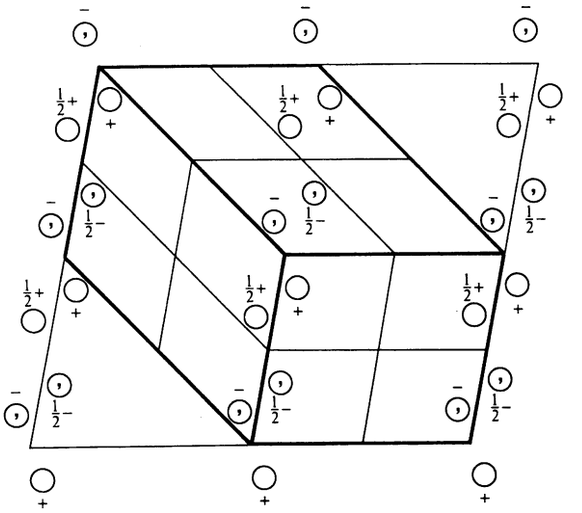
Along [100] $p2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

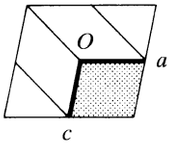
No. 14

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P12_1/c1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at $\bar{1}$

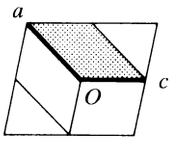
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

$P12_1/n1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$

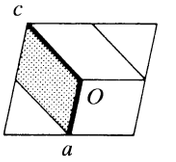
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $h+l=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $h+k+l=2n$
2	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

$P12_1/a1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

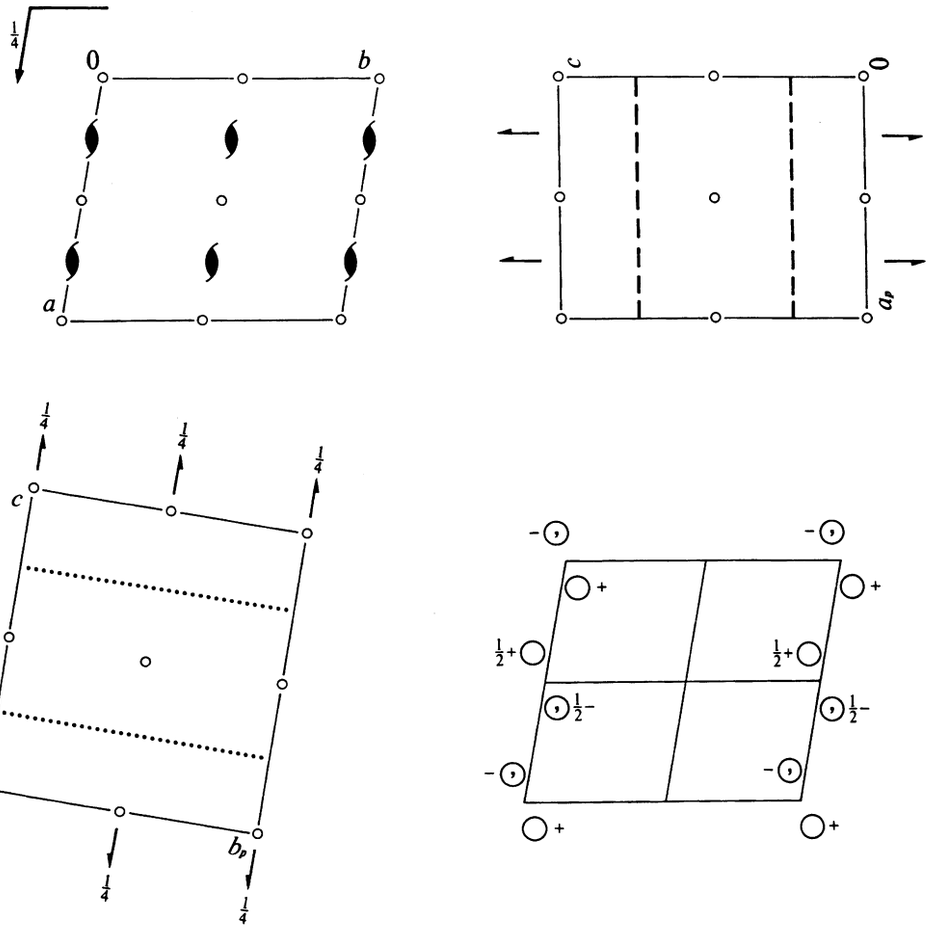
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	$h0l$: $h=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl: $h+k=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

No. 14 $P112_1/a$

Patterson symmetry $P112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $\bar{1}$ $0,0,0$ (4) a $x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$hk0$: $h=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			hkl: $h+l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+l=2n$

Symmetry of special projections

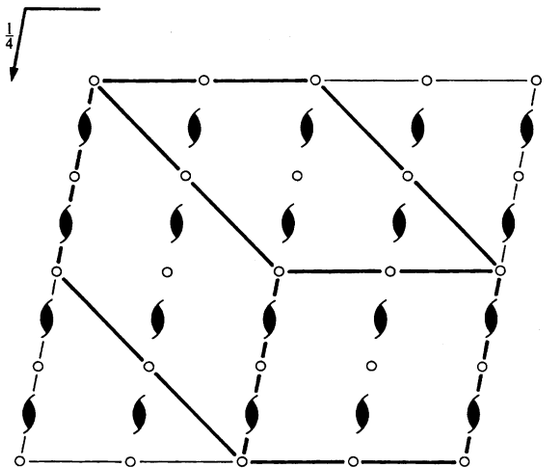
Along [001] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

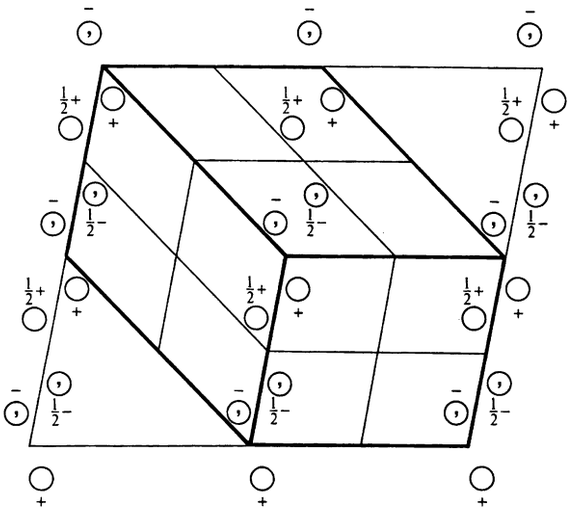
Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}_p$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}_p$
Origin at $0,y,0$

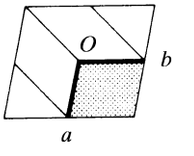
No. 14

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$P112_1/a$



UNIQUE AXIS c, CELL CHOICE 1

Origin at $\bar{1}$

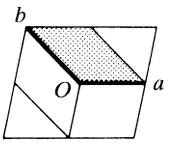
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$hk0$: $h=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			hkl: $h+l=2n$
2	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+l=2n$

$P112_1/n$



UNIQUE AXIS c, CELL CHOICE 2

Origin at $\bar{1}$

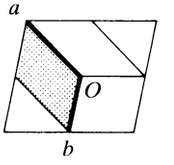
Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$hk0$: $h+k=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
2	d	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	c	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

$P112_1/b$



UNIQUE AXIS c, CELL CHOICE 3

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

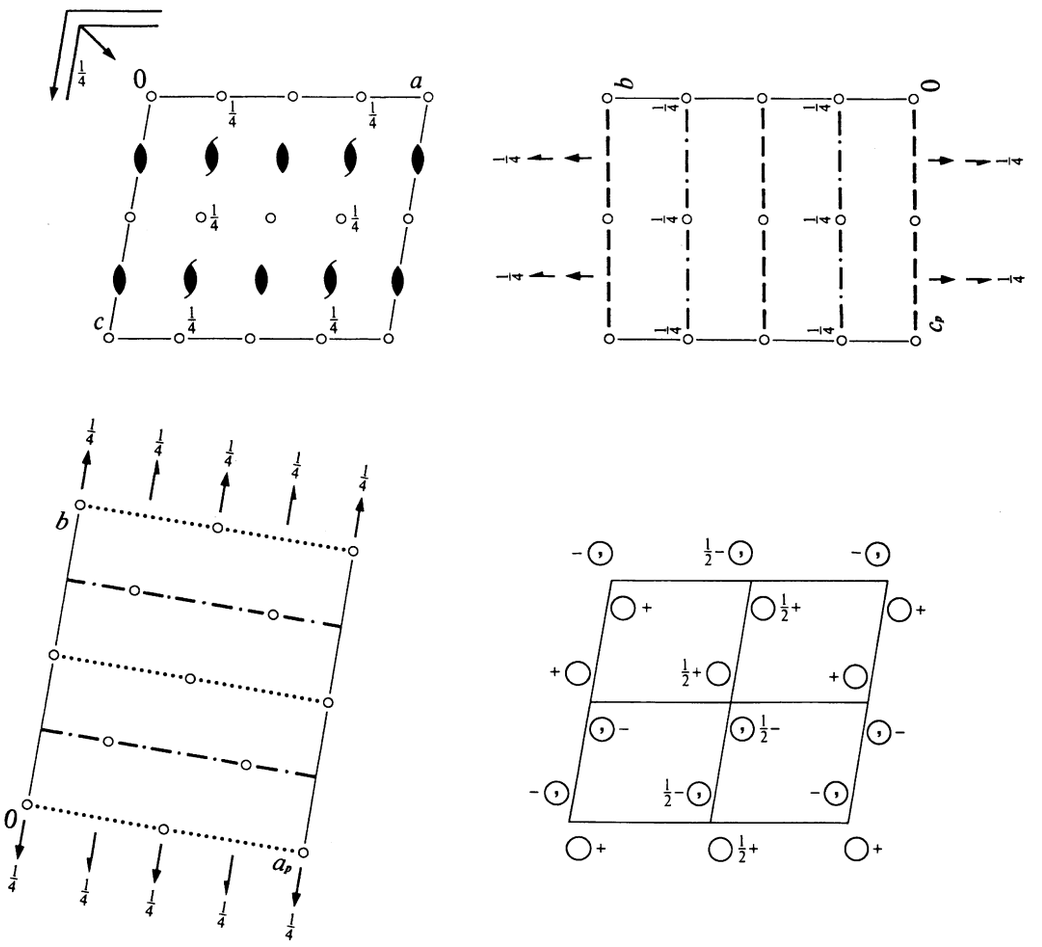
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$hk0$: $k=2n$ $00l$: $l=2n$ $0k0$: $k=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
2	c	$\bar{1}$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			hkl: $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

$C2/c$ C_{2h}^6 $2/m$ Monoclinic

No. 15 $C12/c1$ Patterson symmetry $C12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane c

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,0,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (3) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$ (4) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
8	f	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	hkl: $h+k=2n$ $h0l$: $h,l=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$ $0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$			hkl: $k+l=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

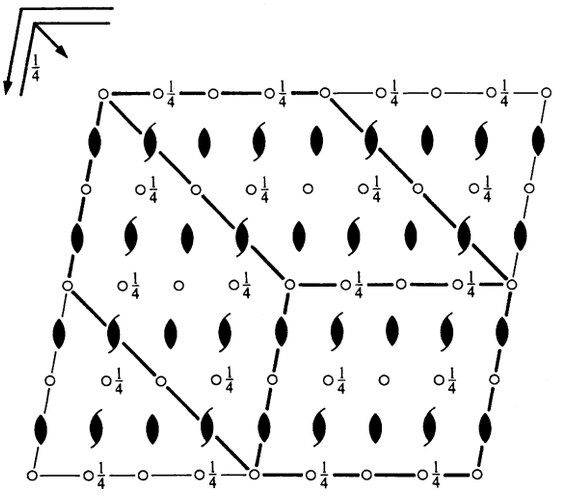
Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

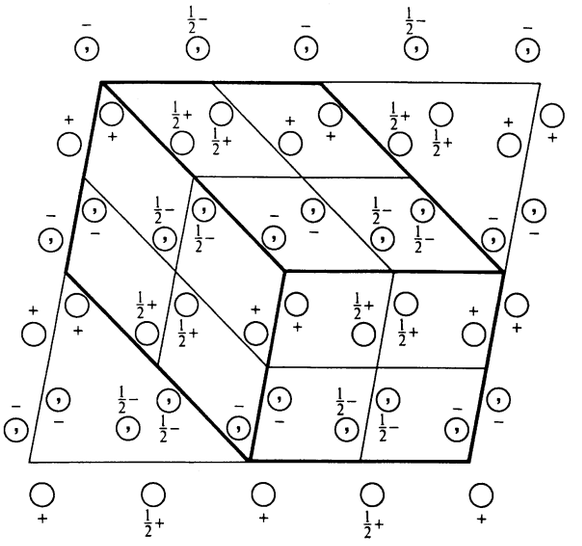
Along [100] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

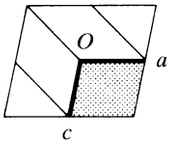
No. 15

UNIQUE AXIS b, DIFFERENT CELL CHOICES





$C12/c1$



UNIQUE AXIS b, CELL CHOICE 1

Origin at $\bar{1}$ on glide plane c

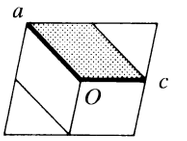
Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions	
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:	
8	f	1	(1) x,y,z	(2) $\bar{x},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y},z+\frac{1}{2}$	hkl: $h+k=2n$ $h0l$: $h,l=2n$ $0kl$: $k=2n$ $hk0$: $h+k=2n$	$0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus	
4	e	2	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions	
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$			hkl: $k+l=2n$	
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$	
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$				
4	a	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$				

$A12/n1$



UNIQUE AXIS b, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

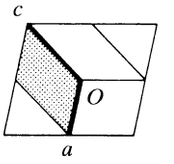
Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions	
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$			General:	
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	hkl: $k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $k=2n$	$0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus	
4	e	2	$\frac{3}{4},y,\frac{3}{4}$	$\frac{1}{4},\bar{y},\frac{1}{4}$			no extra conditions	
4	d	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$0,\frac{1}{4},\frac{3}{4}$			hkl: $h=2n$	
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$	
4	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$				
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$				

$I12/a1$



UNIQUE AXIS b, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

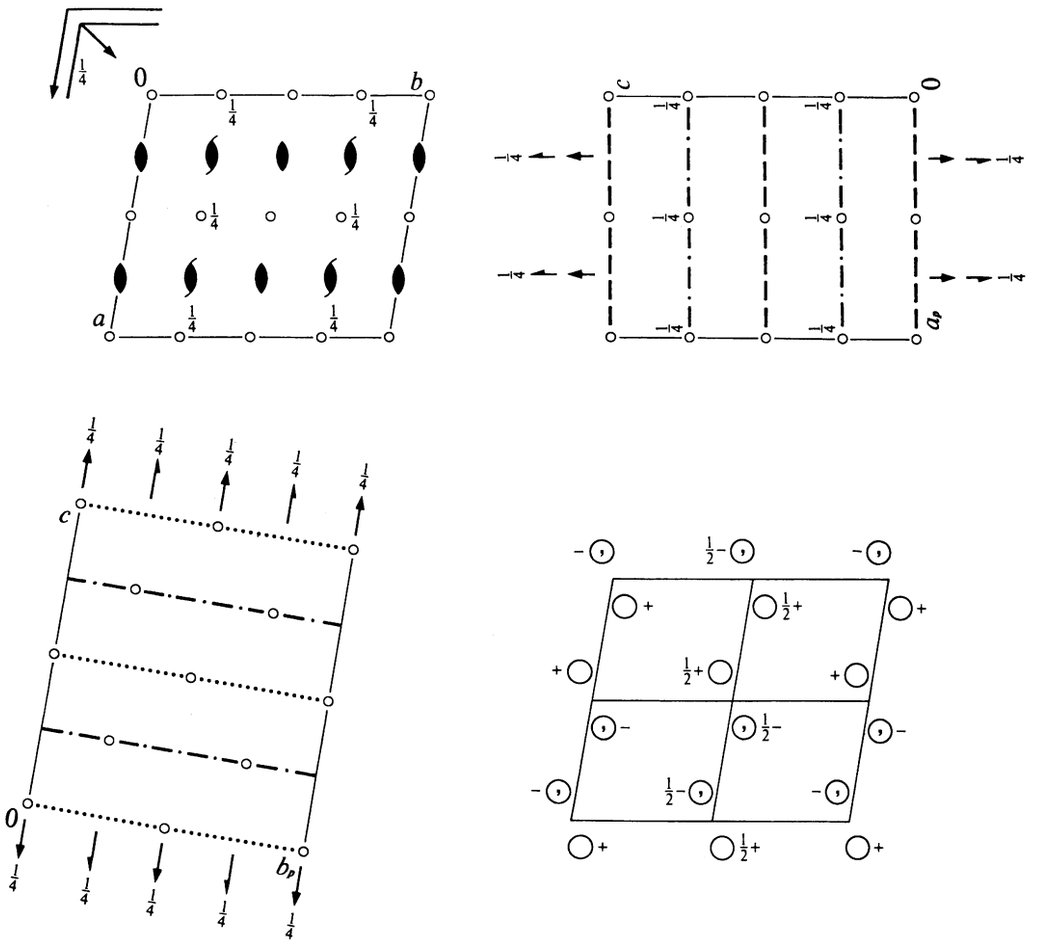
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions	
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:	
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},z$	hkl: $h+k+l=2n$ $h0l$: $h,l=2n$ $0kl$: $k+l=2n$ $hk0$: $h+k=2n$	$0k0$: $k=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus	
4	e	2	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y},0$			no extra conditions	
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			hkl: $l=2n$	
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h=2n$	
4	c	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$				
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$				

No. 15 $A112/a$

Patterson symmetry $A112/m$

UNIQUE AXIS c, CELL CHOICE 1



Origin at $\bar{1}$ on glide plane a

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $\frac{1}{4},0,z$ (3) $\bar{1}$ $0,0,0$ (4) a $x,y,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$ (4) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$			General:
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	hkl: $k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	e	2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl: $h+k=2n$
4	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			hkl: $h+k=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			hkl: $h=2n$

Symmetry of special projections

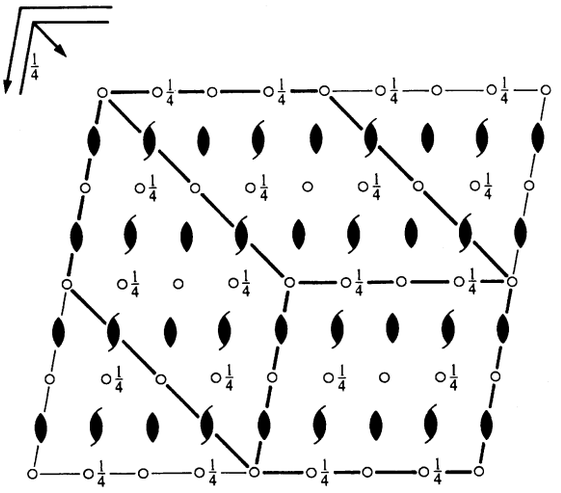
Along [001] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

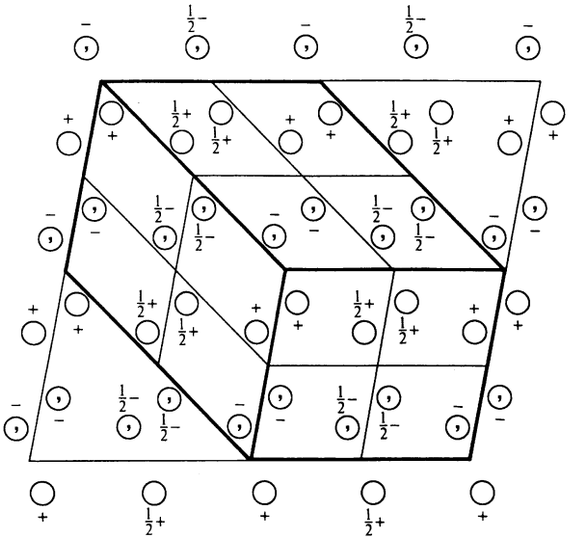
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

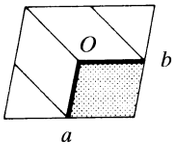
No. 15

UNIQUE AXIS c, DIFFERENT CELL CHOICES





$A112/a$



UNIQUE AXIS c, CELL CHOICE 1

Origin at $\bar{1}$ on glide plane a

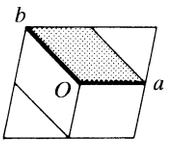
Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
	$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$				General:
8 f 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y,\bar{z}$	hkl: $k+l=2n$ $00l$: $l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0kl$: $k+l=2n$ $0k0$: $k=2n$ $h0l$: $l=2n$
					Special: as above, plus
4 e 2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
4 d $\bar{1}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl: $h+k=2n$
4 b $\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h=2n$
4 c $\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			
4 a $\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$			

$B112/n$



UNIQUE AXIS c, CELL CHOICE 2

Origin at $\bar{1}$ on glide plane n

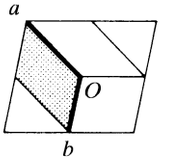
Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},0,\frac{1}{2})+$				Reflection conditions
8	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	General: hkl: $h+l=2n$; $00l$: $l=2n$; $hk0$: $h,k=2n$; $h00$: $h=2n$; $0kl$: $l=2n$; $0k0$: $k=2n$; $h0l$: $h+l=2n$
							Special: as above, plus
4	e	2	$\frac{3}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$			hkl: $k=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
4	c	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$			
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			

$I112/b$



UNIQUE AXIS c, CELL CHOICE 3

Origin at $\bar{1}$ on glide plane b

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

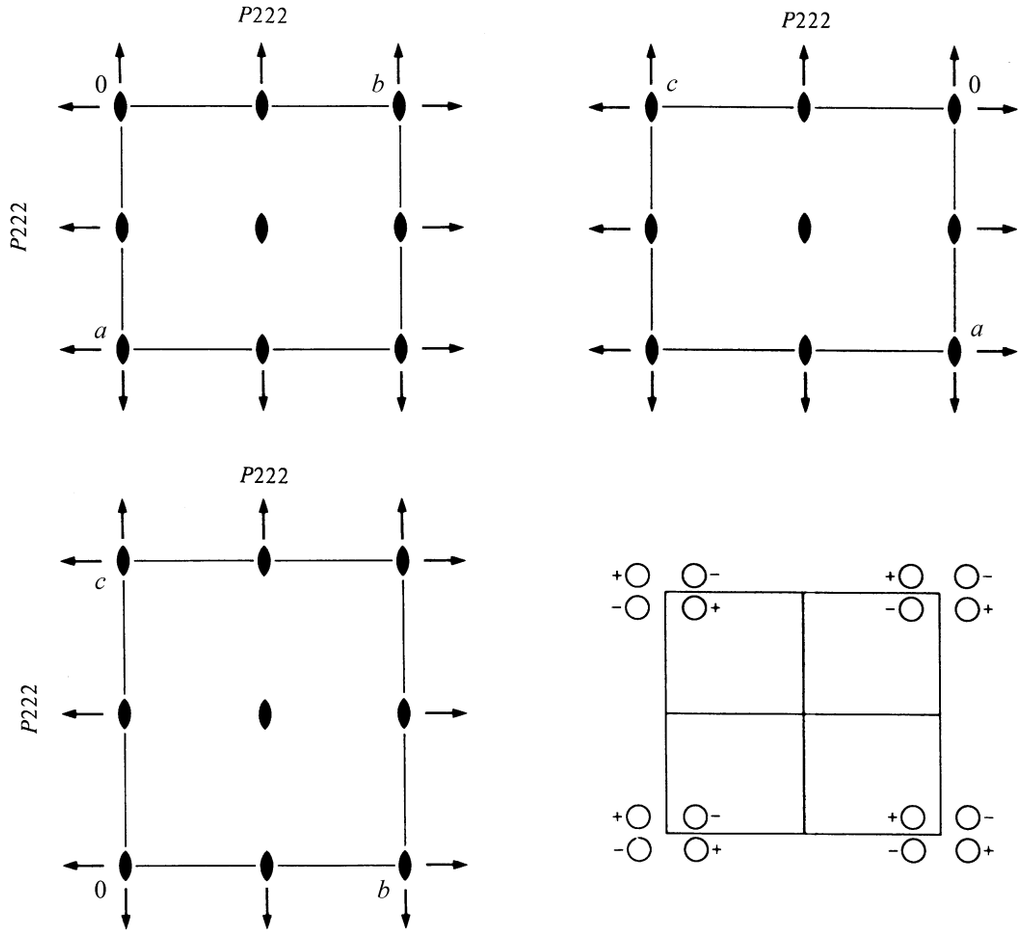
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y+\frac{1}{2},\bar{z}$	General: hkl: $h+k+l=2n$; $00l$: $l=2n$; $hk0$: $h,k=2n$; $h00$: $h=2n$; $0kl$: $k+l=2n$; $0k0$: $k=2n$; $h0l$: $h+l=2n$
							Special: as above, plus
4	e	2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4	d	$\bar{1}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			hkl: $h=2n$
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k=2n$
4	c	$\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$			
4	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},0$			

$P222$ D_2^1 222 Orthorhombic

No. 16 $P222$ Patterson symmetry $Pmmm$



Origin at 222

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	u	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	no conditions
							Special: no extra conditions
2	t	. . 2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	s	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	r	. . 2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	q	. . 2	$0,0,z$	$0,0,\bar{z}$			
2	p	. 2 .	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$			
2	o	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	n	. 2 .	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	m	. 2 .	$0,y,0$	$0,\bar{y},0$			
2	l	2 . .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$			
2	k	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			
2	j	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
2	i	2 . .	$x,0,0$	$\bar{x},0,0$			
1	h	2 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	2 2 2	$0,\frac{1}{2},\frac{1}{2}$				
1	f	2 2 2	$\frac{1}{2},0,\frac{1}{2}$				
1	e	2 2 2	$\frac{1}{2},\frac{1}{2},0$				
1	d	2 2 2	$0,0,\frac{1}{2}$				
1	c	2 2 2	$0,\frac{1}{2},0$				
1	b	2 2 2	$\frac{1}{2},0,0$				
1	a	2 2 2	$0,0,0$				

Symmetry of special projections

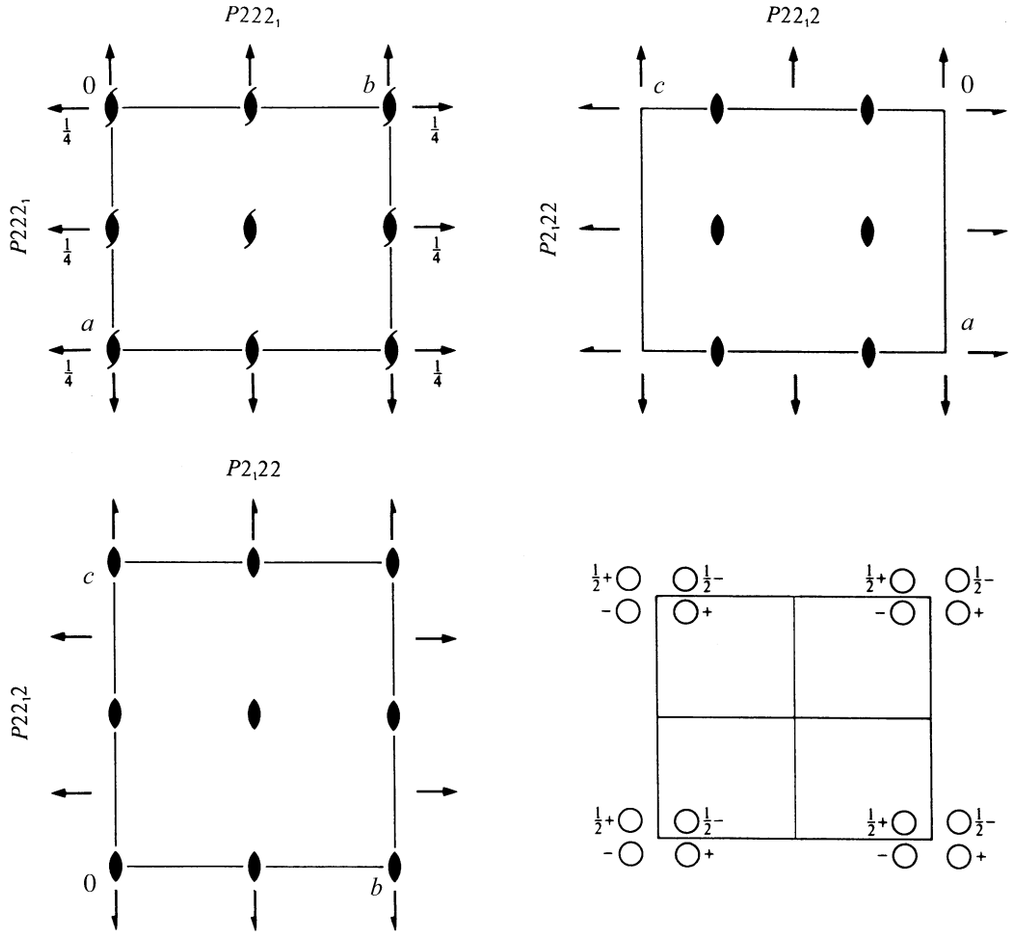
Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

$P222_1$ D_2^2 222 Orthorhombic

No. 17 $P222_1$ Patterson symmetry $Pmmm$



Origin at $2\,1\,2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) 2 $0,y,\frac{1}{4}$ (4) 2 $x,0,0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$	$00l$: $l=2n$
							Special: as above, plus
2	d	. 2 .	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$			$h0l$: $l=2n$
2	c	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			$h0l$: $l=2n$
2	b	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},\frac{1}{2}$			$0kl$: $l=2n$
2	a	2 . .	$x,0,0$	$\bar{x},0,\frac{1}{2}$			$0kl$: $l=2n$

Symmetry of special projections

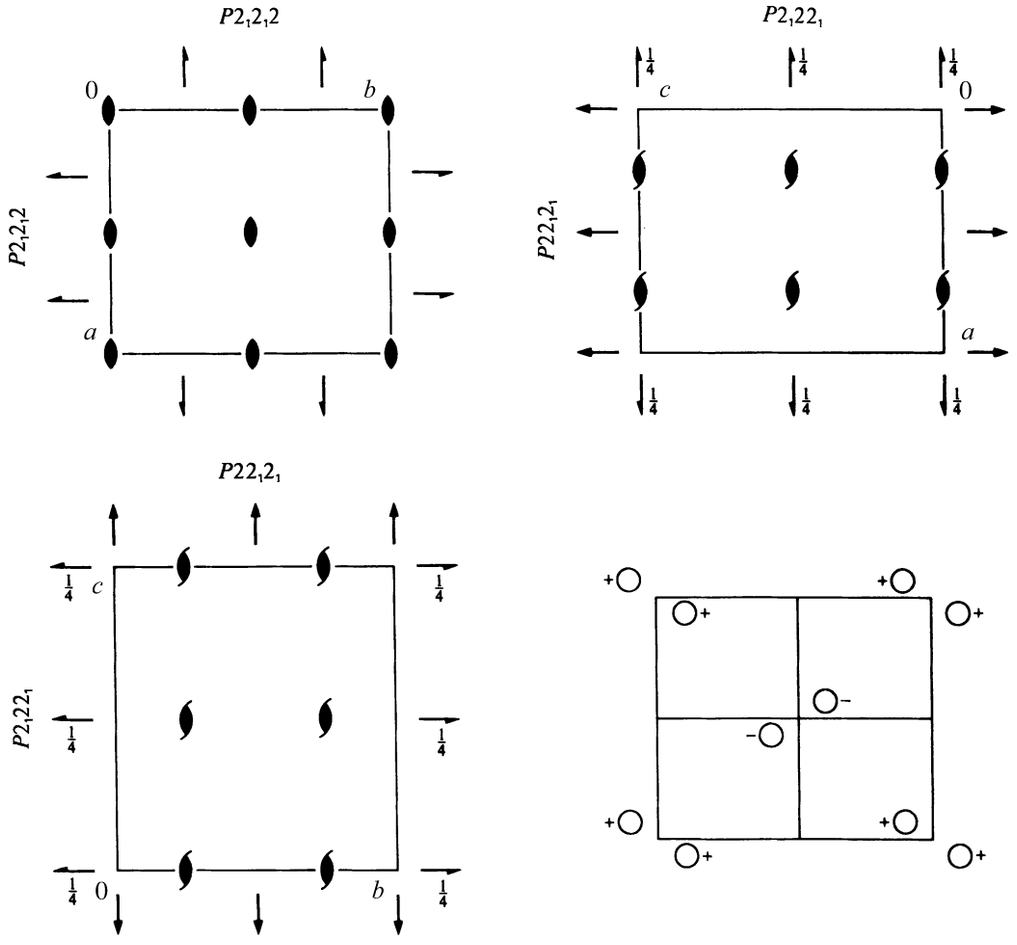
Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,\frac{1}{4}$

$P2_12_12$ D_2^3 222 Orthorhombic

No. 18 $P2_12_12$ Patterson symmetry $Pmmm$



Origin at intersection of 2 with perpendicular plane containing 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 c 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$ $0k0$: $k=2n$
					Special: as above, plus
2 b . . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2 a . . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			$hk0$: $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $p2gm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $\frac{1}{4},y,0$

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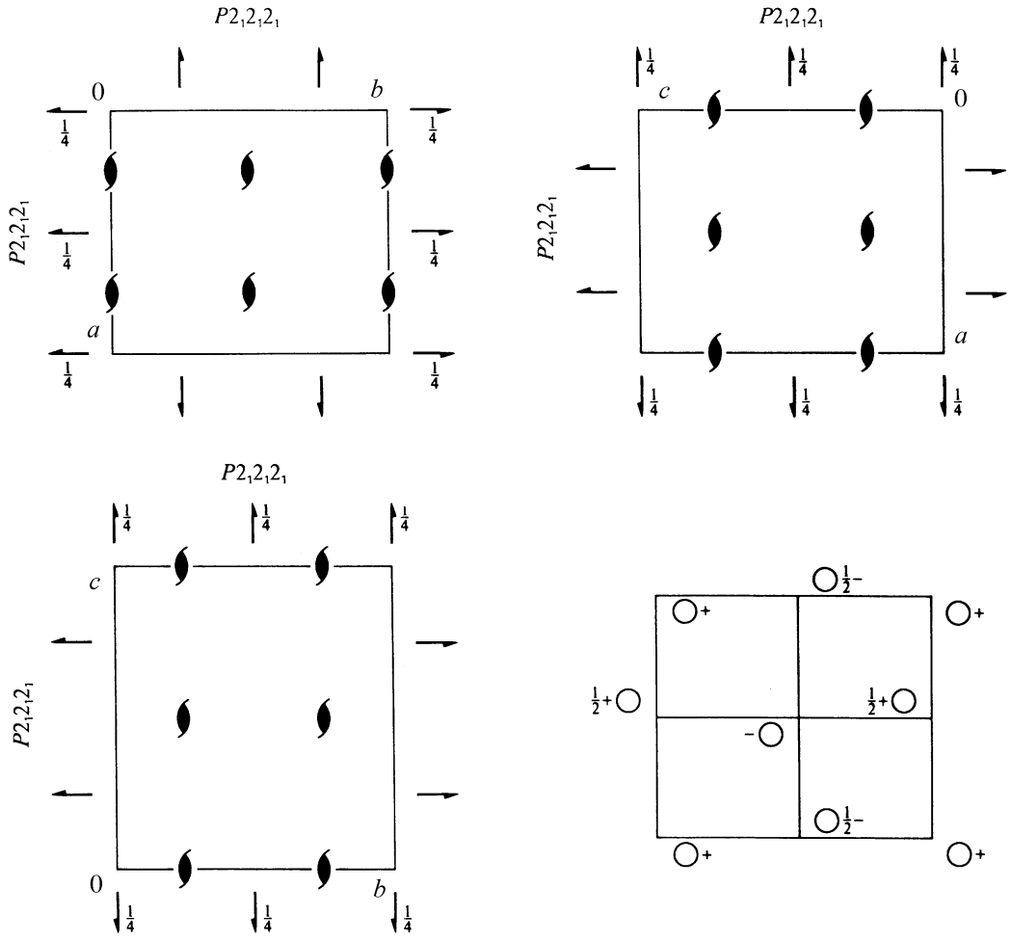
Orthorhombic 222 D_2^4 $P2_12_12_1$

Patterson symmetry $Pmmm$ $P2_12_12_1$ No. 19



Origin at midpoint of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $p2gg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $p2gg$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,\frac{1}{4}$

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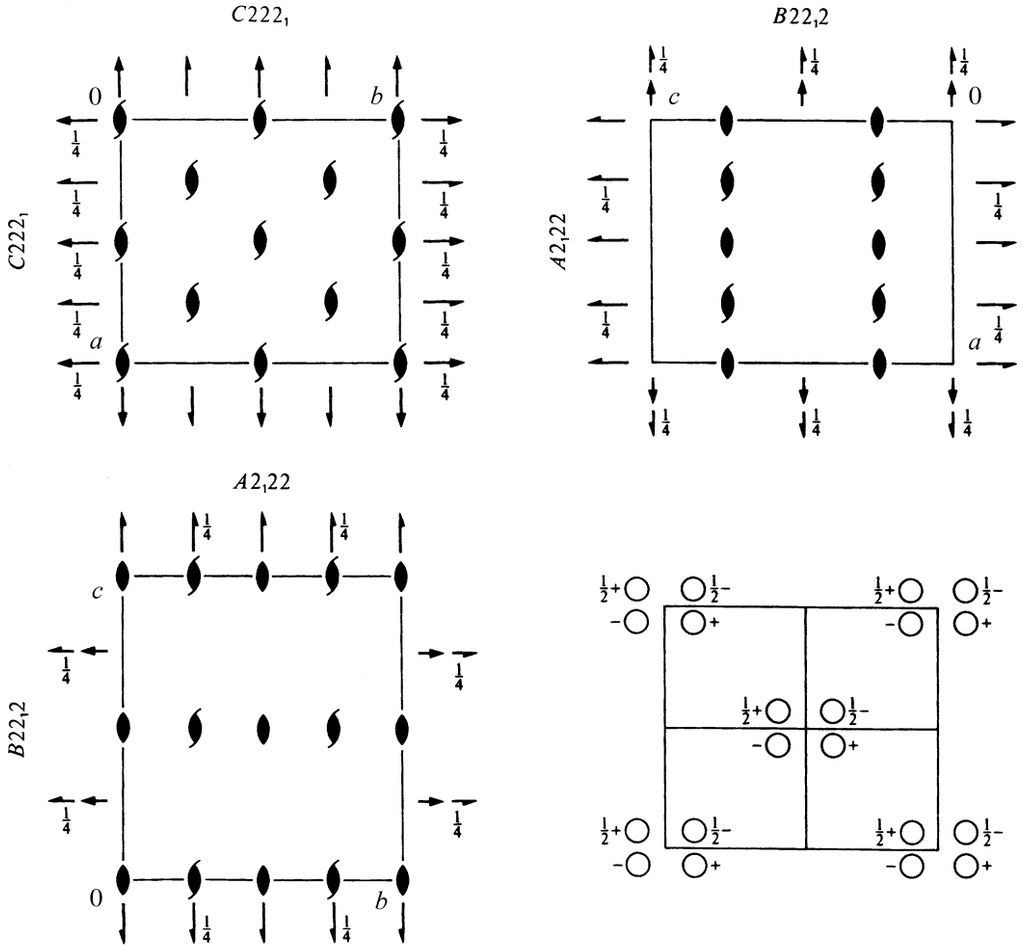
International Tables for Crystallography (2016). Vol. A, Space group 20, pp. 274–275.

$C222_1$ D_2^5 222 Orthorhombic

No. 20 $C222_1$ Patterson symmetry $Cmmm$



Origin at $2\,1\,2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) 2 $0,y,\frac{1}{4}$ (4) 2 $x,0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			Reflection conditions
						General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (4) $x,\bar{y},\bar{z}$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
						Special: as above, plus
4	b	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$		$h0l$: $l=2n$
4	a	2 . .	$x,0,0$	$\bar{x},0,\frac{1}{2}$		$0kl$: $l=2n$

Symmetry of special projections

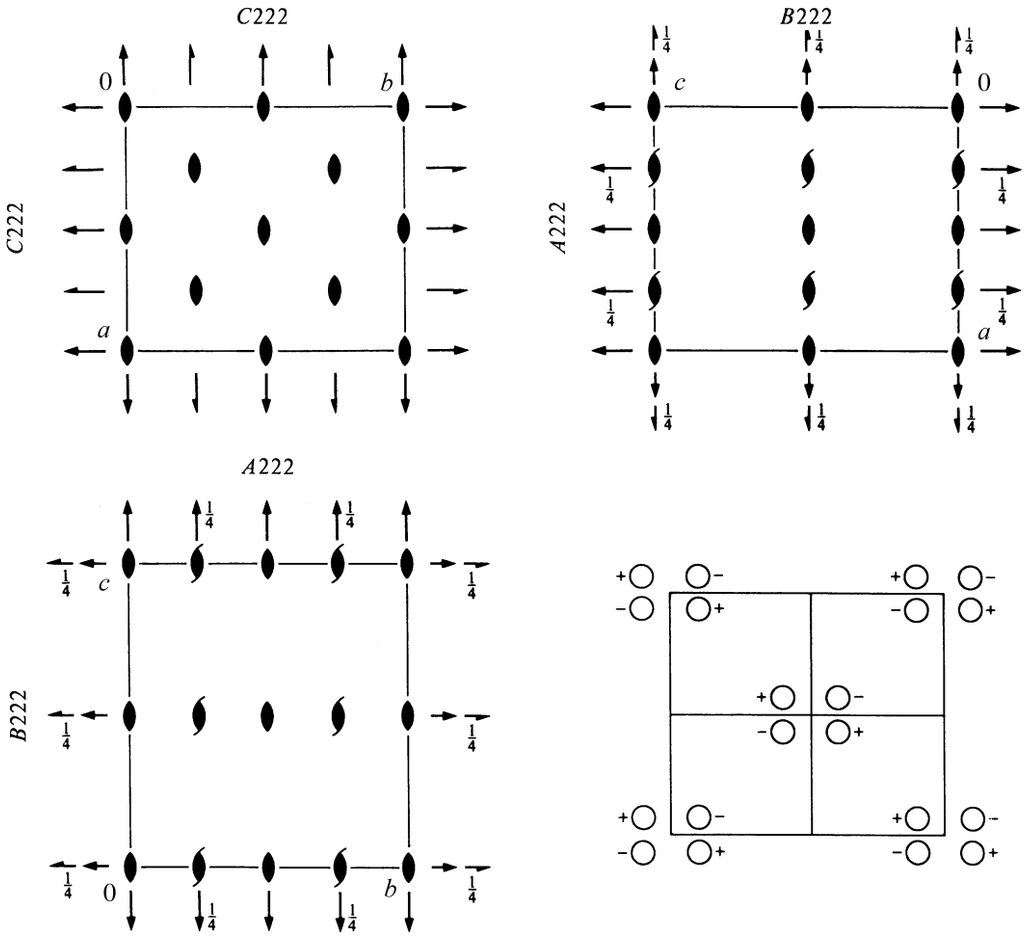
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,\frac{1}{4}$

$C222$ D_2^6 222 Orthorhombic

No. 21 $C222$ Patterson symmetry $Cmmm$



Origin at 222

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	*l*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	*hkl*: $h+k=2n$ *hk*0: $h+k=2n$ 0*kl*: $k=2n$ *h*00: $h=2n$ *h*0*l*: $h=2n$ 0*k*0: $k=2n$
							Special: as above, plus
4	*k*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			*hk*0: $h=2n$
4	*j*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	*i*	. . 2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	*h*	. 2 .	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	*g*	. 2 .	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	*f*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			no extra conditions
4	*e*	2 . .	$x,0,0$	$\bar{x},0,0$			no extra conditions
2	*d*	2 2 2	$0,0,\frac{1}{2}$				no extra conditions
2	*c*	2 2 2	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	*b*	2 2 2	$0,\frac{1}{2},0$				no extra conditions
2	*a*	2 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

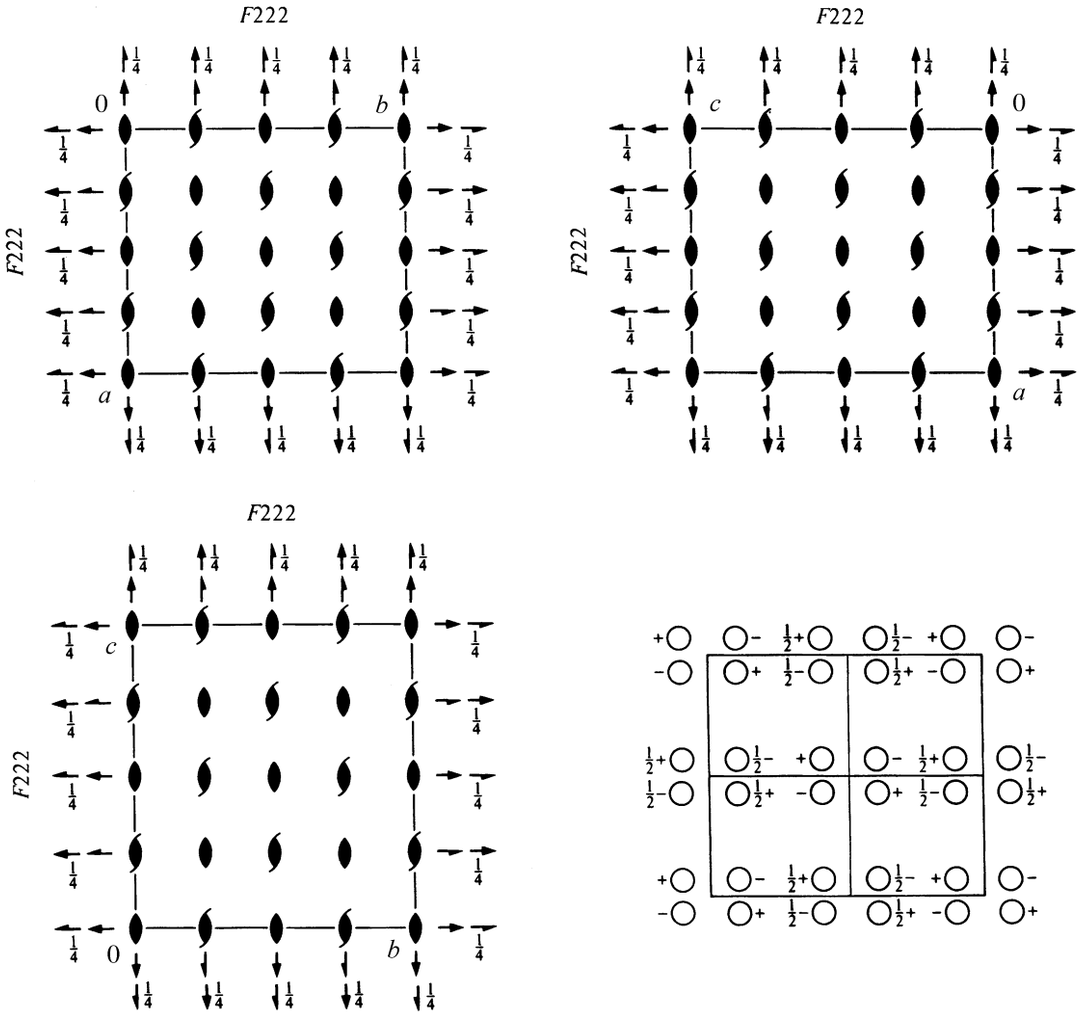
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$F222$ D_2^7 222 Orthorhombic

No. 22 $F222$ Patterson symmetry $Fmmm$



Origin at 222

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (4) 2 $x,\frac{1}{4},\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) 2 $\frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl: $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: no extra conditions
8	j	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$			
8	i	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{1}{4}$			
8	h	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			
8	g	. . 2	$0,0,z$	$0,0,\bar{z}$			
8	f	. 2 .	$0,y,0$	$0,\bar{y},0$			
8	e	2 . .	$x,0,0$	$\bar{x},0,0$			
4	d	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$				
4	c	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$				
4	b	2 2 2	$0,0,\frac{1}{2}$				
4	a	2 2 2	$0,0,0$				

Symmetry of special projections

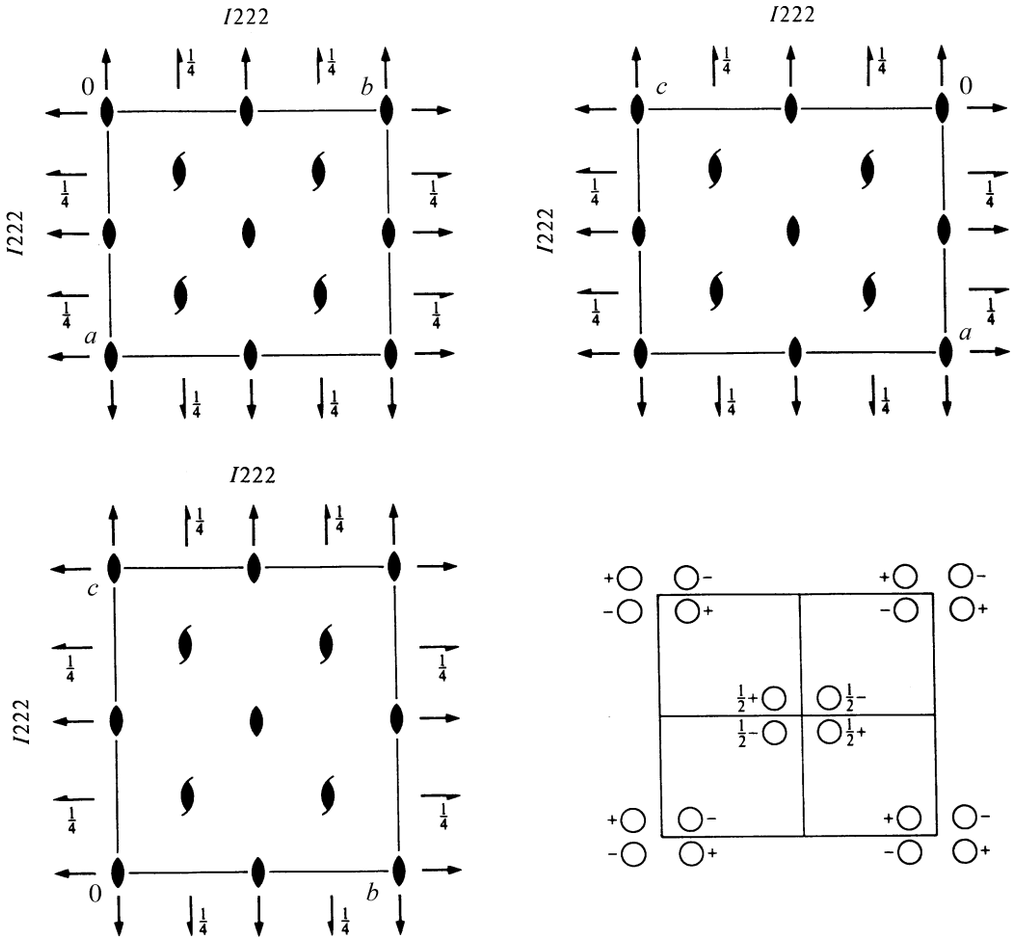
Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$I222$ D_2^8 222 Orthorhombic

No. 23 $I222$ Patterson symmetry $Immm$



Origin at 222

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) 2 $0,y,0$ (4) 2 $x,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
8	*k*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
4	*j*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$		
4	*i*	. . 2	$0,0,z$	$0,0,\bar{z}$		
4	*h*	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$		
4	*g*	. 2 .	$0,y,0$	$0,\bar{y},0$		
4	*f*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$		
4	*e*	2 . .	$x,0,0$	$\bar{x},0,0$		
2	*d*	2 2 2	$0,\frac{1}{2},0$			
2	*c*	2 2 2	$0,0,\frac{1}{2}$			
2	*b*	2 2 2	$\frac{1}{2},0,0$			
2	*a*	2 2 2	$0,0,0$			

Reflection conditions

General:

hkl: $h+k+l=2n$
0*kl*: $k+l=2n$
*h*0*l*: $h+l=2n$
*hk*0: $h+k=2n$
*h*00: $h=2n$
0*k*0: $k=2n$
00*l*: $l=2n$

Special: no extra conditions

Symmetry of special projections

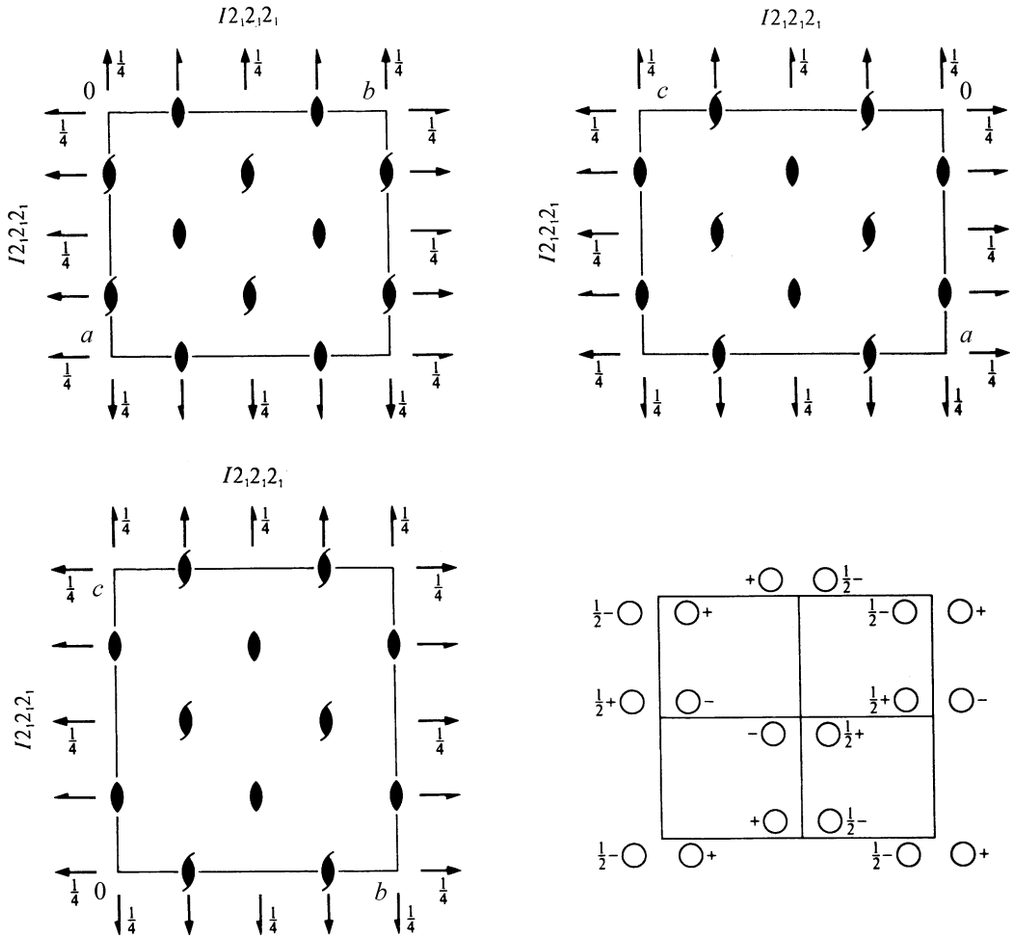
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$I2_12_12_1$ D_2^9 222 Orthorhombic

No. 24 $I2_12_12_1$ Patterson symmetry $Immm$



Origin at midpoint of three non-intersecting pairs of parallel 2 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) 2 $0,\frac{1}{4},z$ (3) 2 $\frac{1}{4},y,0$ (4) 2 $x,0,\frac{1}{4}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	c	. . 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}+\frac{1}{2}$			$hk0$: $h=2n$
4	b	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},\frac{1}{2}$			$h0l$: $h=2n$
4	a	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$			$0kl$: $k=2n$

Symmetry of special projections

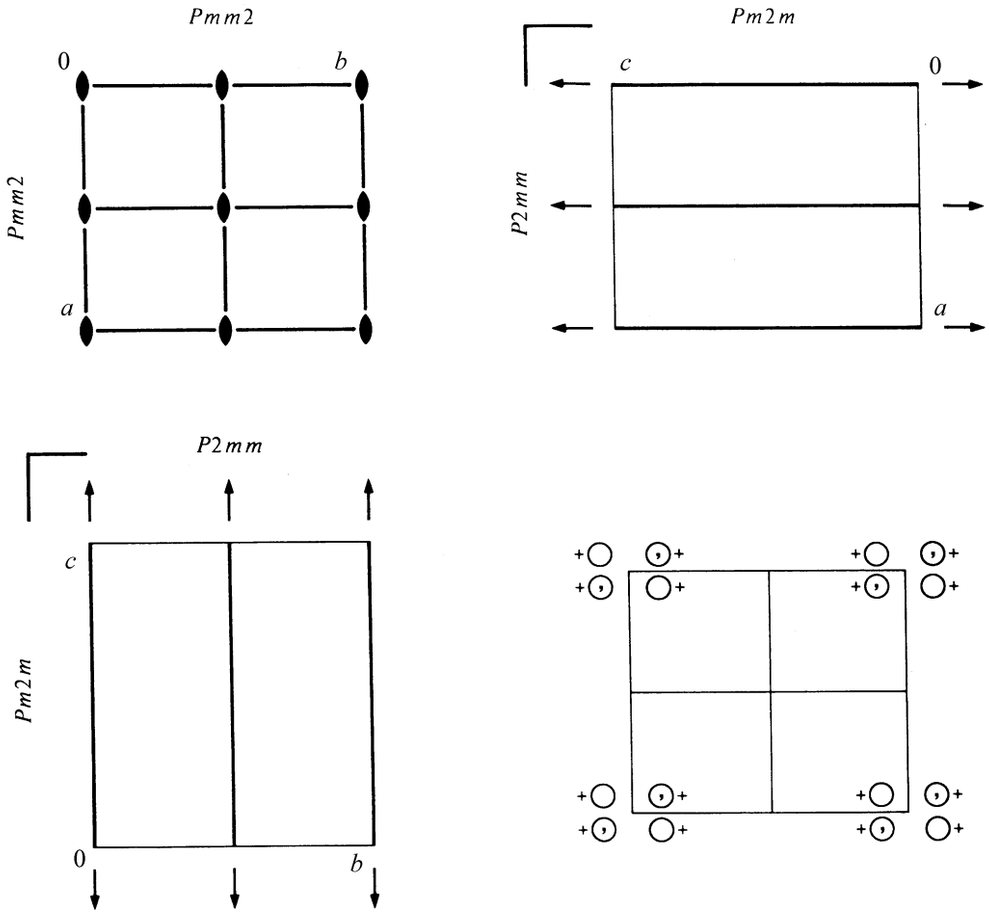
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,\frac{1}{4}$

$Pmm2$ C_{2v}^1 $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$



Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	General: no conditions
							Special: no extra conditions
2	h	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
2	g	m . .	$0,y,z$	$0,\bar{y},z$			
2	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	e	. m .	$x,0,z$	$\bar{x},0,z$			
1	d	$m\,m\,2$	$\frac{1}{2},\frac{1}{2},z$				
1	c	$m\,m\,2$	$\frac{1}{2},0,z$				
1	b	$m\,m\,2$	$0,\frac{1}{2},z$				
1	a	$m\,m\,2$	$0,0,z$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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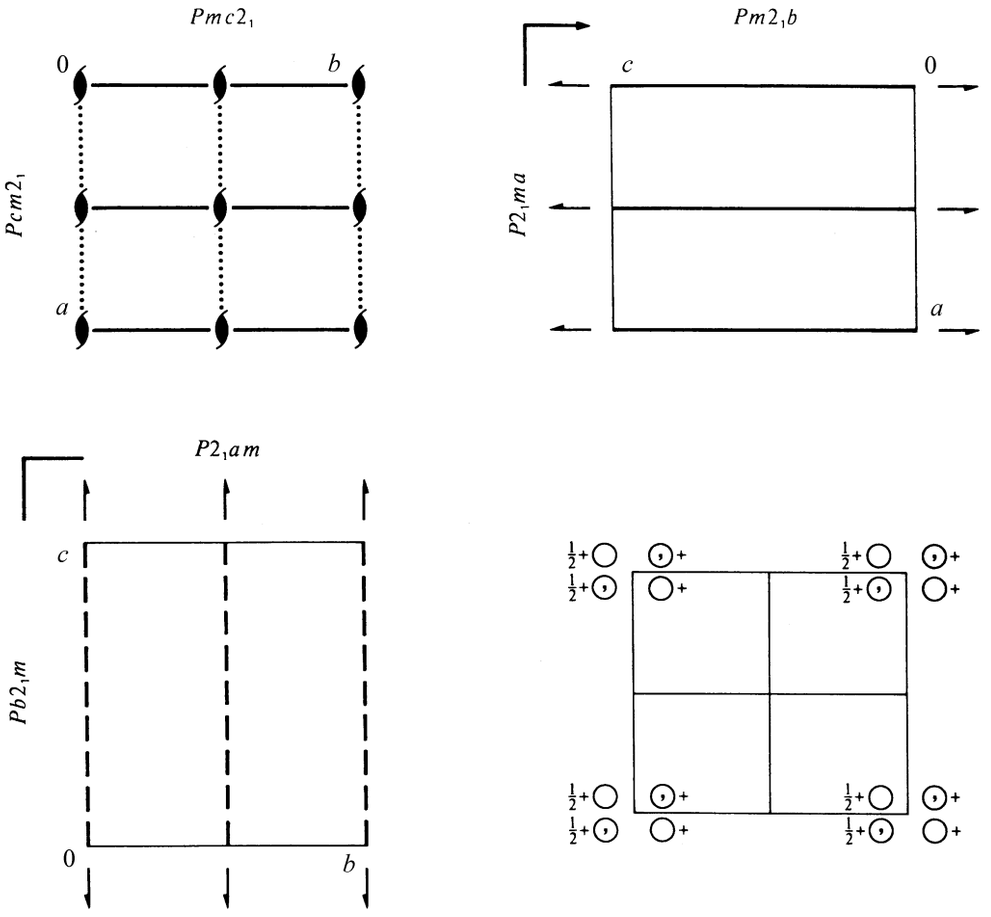
Orthorhombic $mm2$ C_{2v}^2 $Pmc2_1$

Patterson symmetry $Pmmm$ $Pmc2_1$ No. 26



Origin on $mc2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) c $x,0,z$ (4) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z$	$h0l$: $l=2n$ $00l$: $l=2n$
							Special: no extra conditions
2	b	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z+\frac{1}{2}$			
2	a	m . .	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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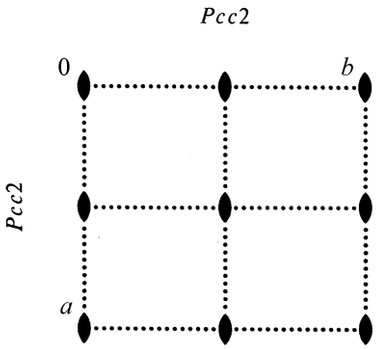
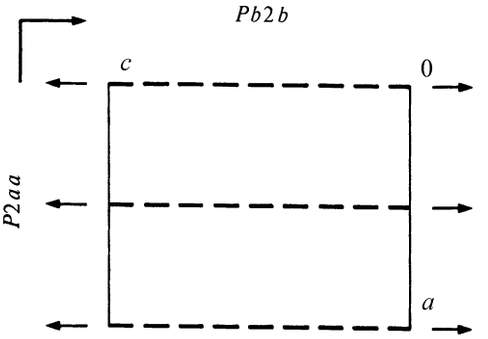
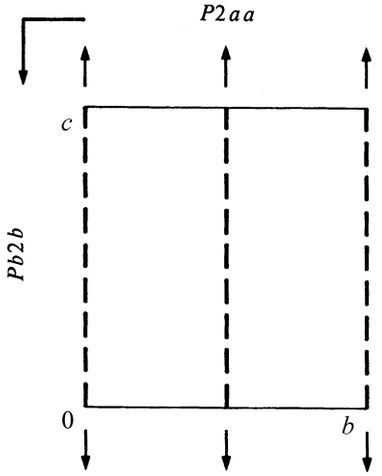
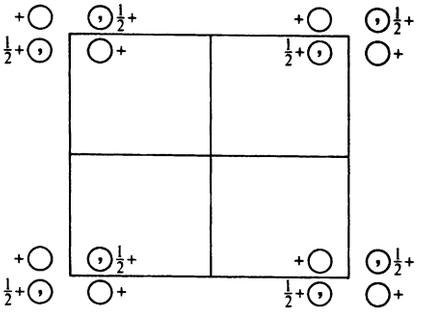
$Pcc2$ C_{2v}^3 $mm2$ Orthorhombic

No. 27 $Pcc2$ Patterson symmetry $Pmmm$









Origin on $cc2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) c $x,0,z$ (4) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 e 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$
					Special: as above, plus
2 d . . 2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $l=2n$
2 c . . 2	$\frac{1}{2},0,z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl: $l=2n$
2 b . . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$			hkl: $l=2n$
2 a . . 2	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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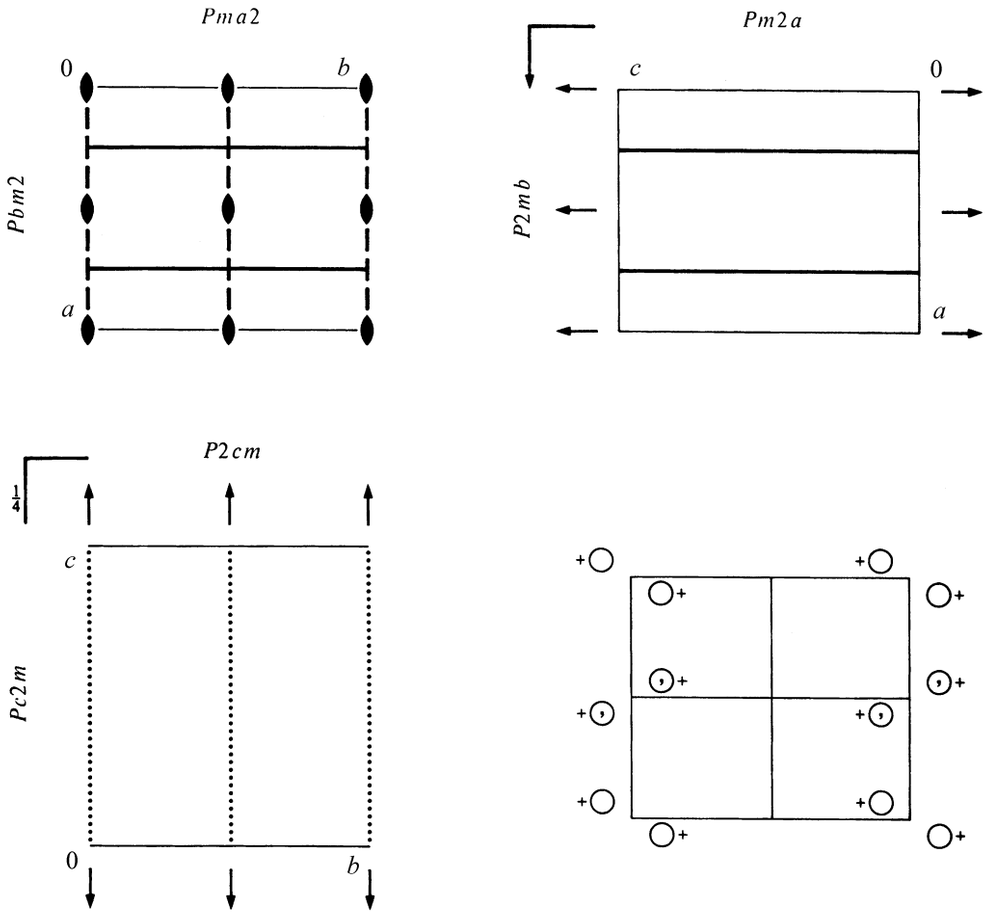
Orthorhombic $mm2$ C_{2v}^4 $Pma2$

Patterson symmetry $Pmmm$ $Pma2$ No. 28



Origin on $1a2$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le 1$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) a $x,0,z$ (4) m $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 d 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	$h0l$: $h=2n$ $h00$: $h=2n$
					Special: as above, plus
2 c m . .	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			no extra conditions
2 b . . 2	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$			hkl: $h=2n$
2 a . . 2	$0,0,z$	$\frac{1}{2},0,z$			hkl: $h=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

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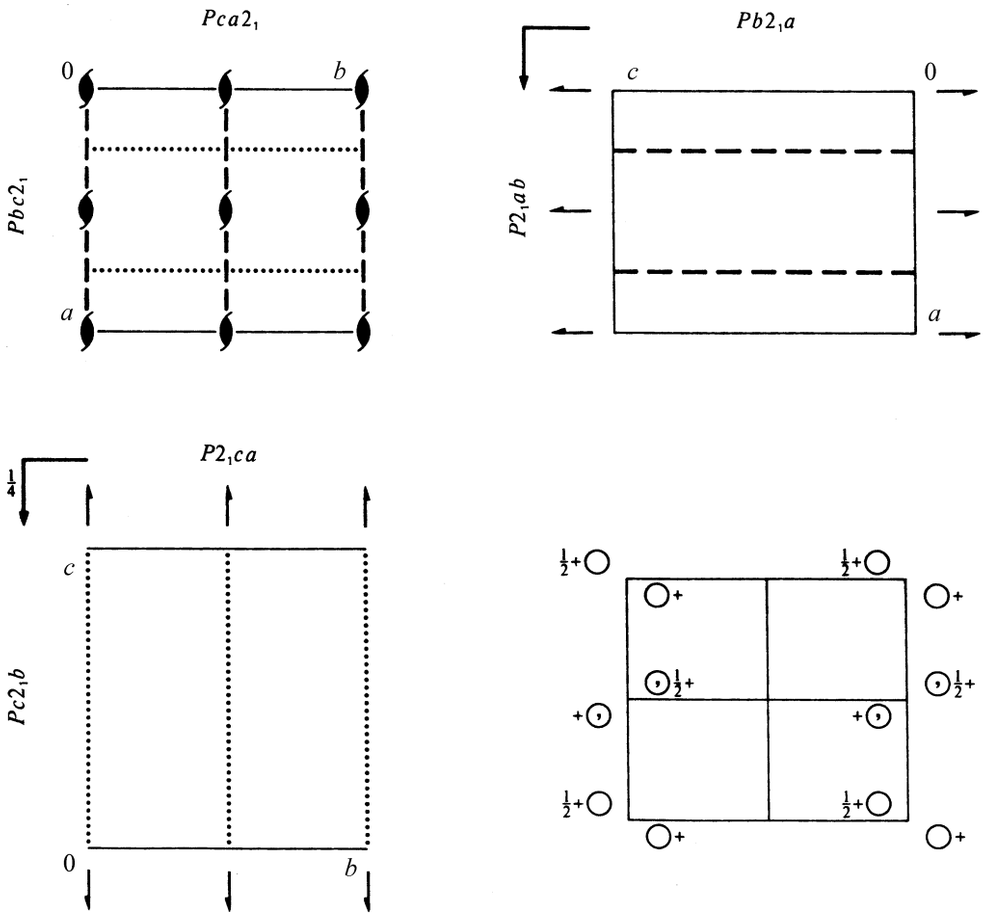
$Pca2_1$ C_{2v}^5 $mm2$ Orthorhombic

No. 29 $Pca2_1$ Patterson symmetry $Pmmm$



Origin on $1a2_1$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le 1$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) a $x,0,z$ (4) c $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11g$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

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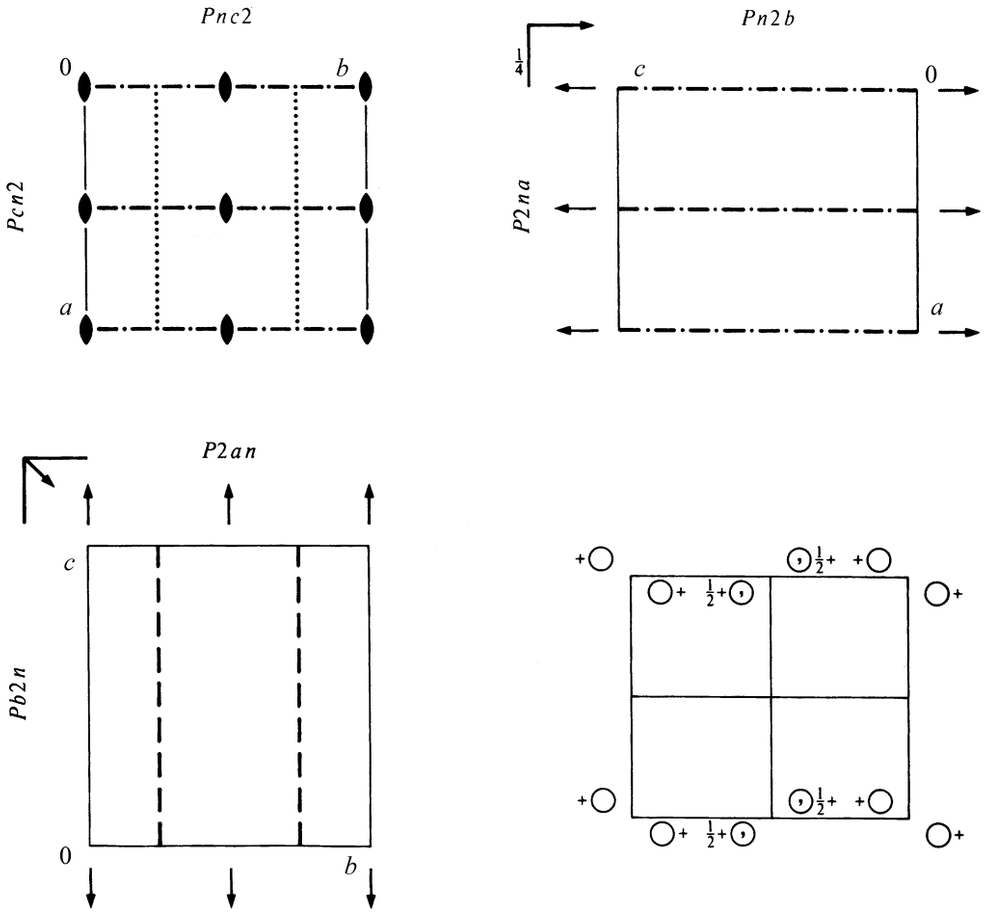
Orthorhombic $mm2$ C_{2v}^6 $Pnc2$

Patterson symmetry $Pmmm$ $Pnc2$ No. 30



Origin on $n12$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) c $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 c 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
					Special: as above, plus
2 b . . 2	$\frac{1}{2},0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $k+l=2n$
2 a . . 2	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{2}$			hkl: $k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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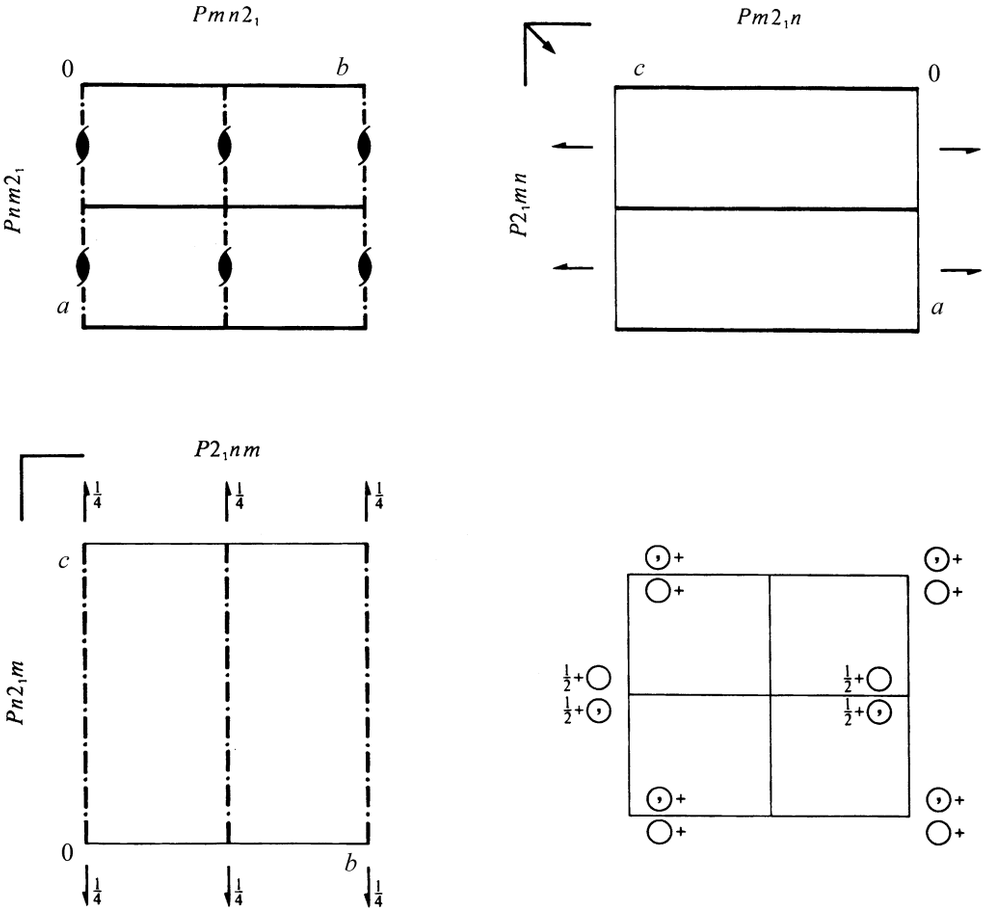
$Pmn2_1$ C_{2v}^7 $mm2$ Orthorhombic

No. 31 $Pmn2_1$ Patterson symmetry $Pmmm$



Origin on $mn1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$ (4) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 b 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z$	$h0l$: $h+l=2n$ $h00$: $h=2n$ $00l$: $l=2n$
					Special: no extra conditions
2 a m . .	$0,y,z$	$\frac{1}{2},\bar{y},z+\frac{1}{2}$			

Symmetry of special projections

Along [001] $p2mg$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $c11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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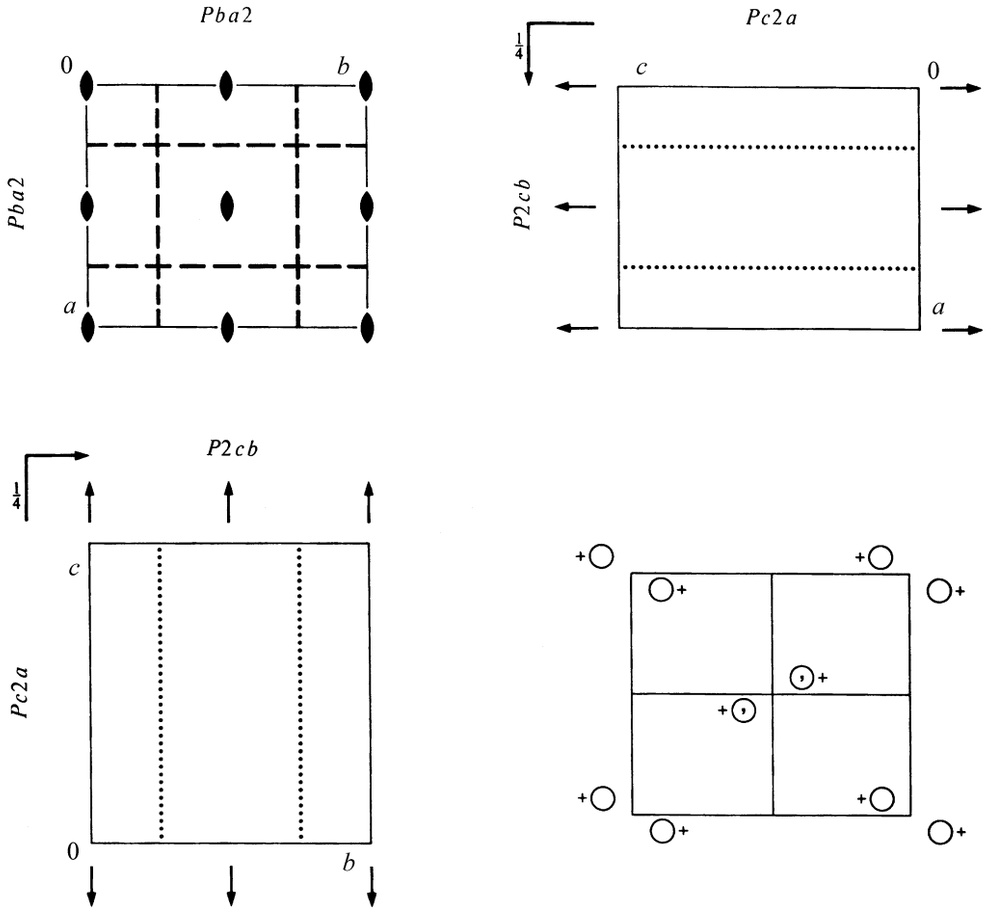
Orthorhombic $mm2$ C_{2v}^{8} $Pba2$

Patterson symmetry $Pmmm$ $Pba2$ No. 32



Origin on 1 1 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 c 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
					Special: as above, plus
2 b . . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl: $h+k=2n$
2 a . . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

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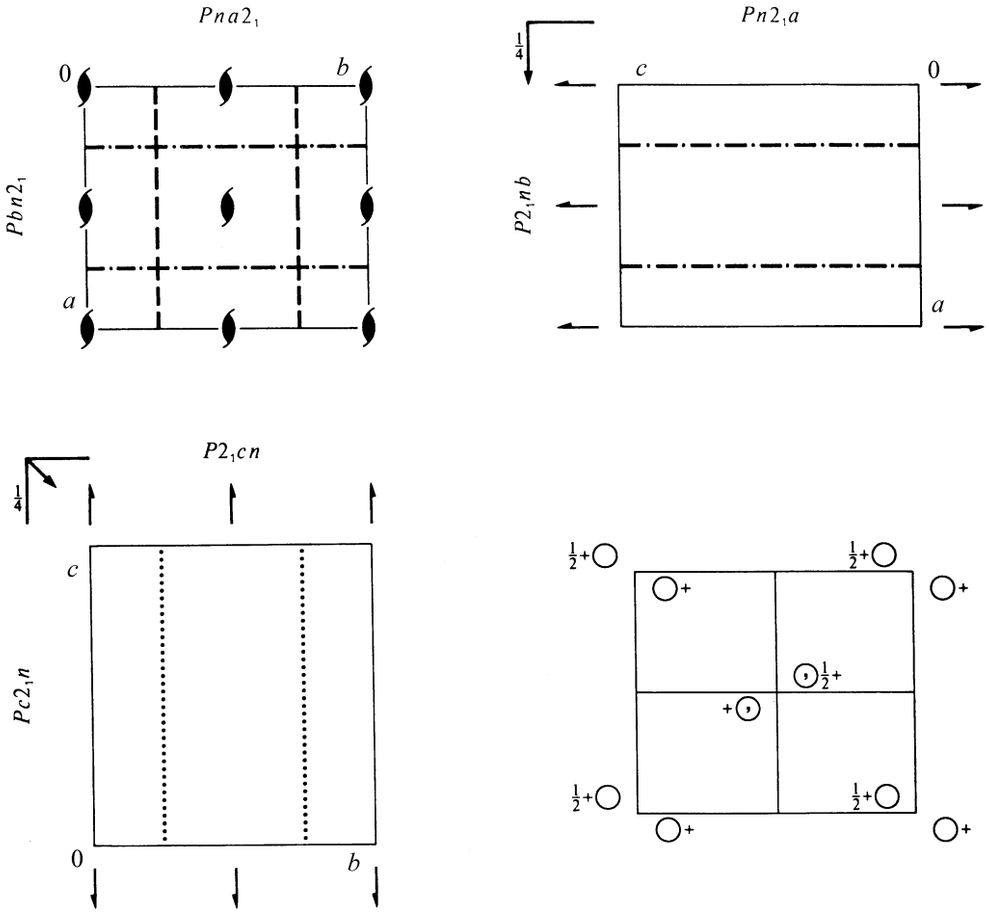
$Pna2_1$ C_{2v}^9 $mm2$ Orthorhombic

No. 33 $Pna2_1$ Patterson symmetry $Pmmm$



Origin on $1\,1\,2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) a $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$

Symmetry of special projections

Along [001] $p\,2\,g\,g$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $p\,1\,1\,g$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

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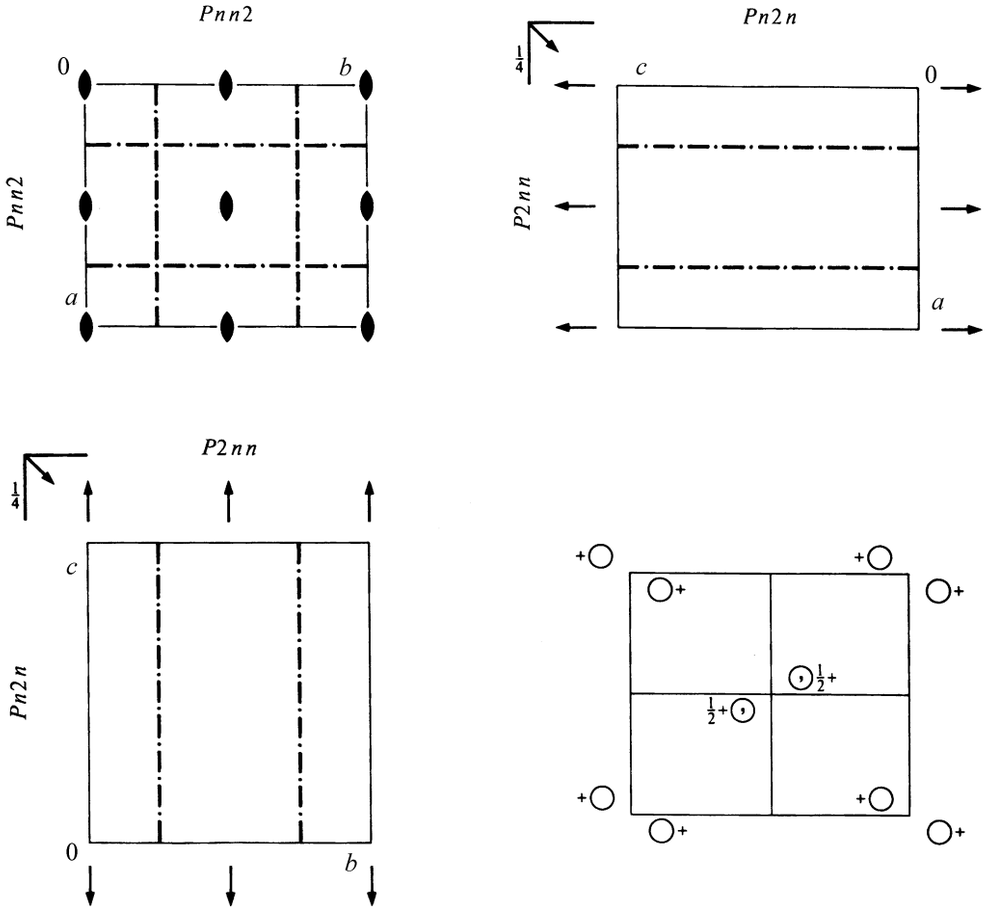
Orthorhombic $mm2$ C_{2v}^{10} $Pnn2$

Patterson symmetry $Pmmm$ $Pnn2$ No. 34



Origin on 1 1 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	b	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl: $h+k+l=2n$
2	a	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p\,2\,g\,g$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $c\,1\,1\,m$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

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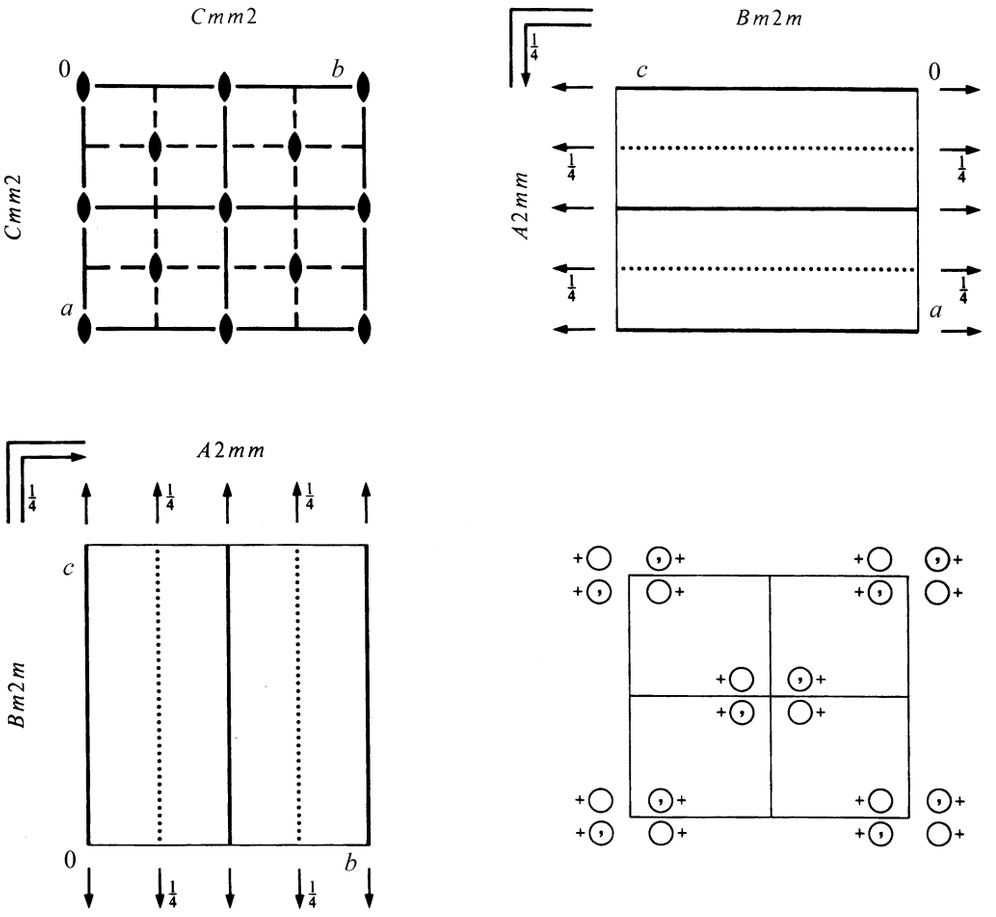
$Cmm2$ C_{2v}^{11} $mm2$ Orthorhombic

No. 35 $Cmm2$ Patterson symmetry $Cmmm$



Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
8	*f*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*e*	*m* . .	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	*d*	. *m* .	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	*c*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl: $h=2n$
2	*b*	*m m* 2	$0,\frac{1}{2},z$				no extra conditions
2	*a*	*m m* 2	$0,0,z$				no extra conditions

Symmetry of special projections

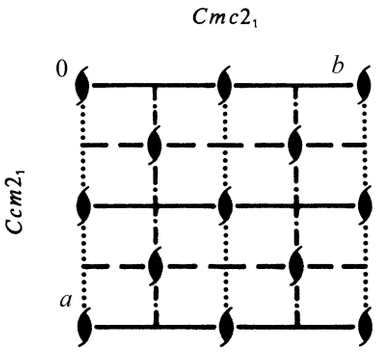
Along [001] *c* 2 *m m*
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

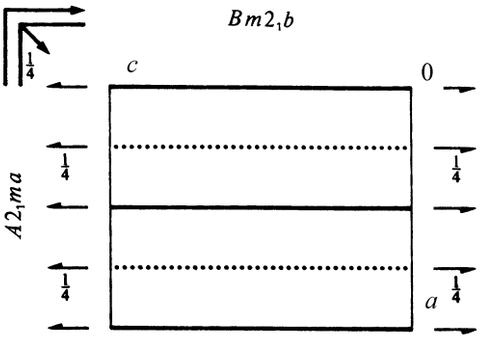
Along [100] *p* 1 *m* 1
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

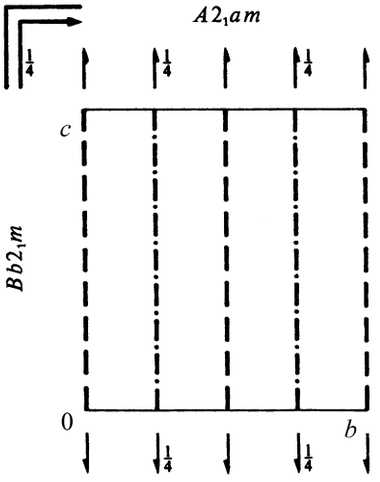
Along [010] *p* 1 1 *m*
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

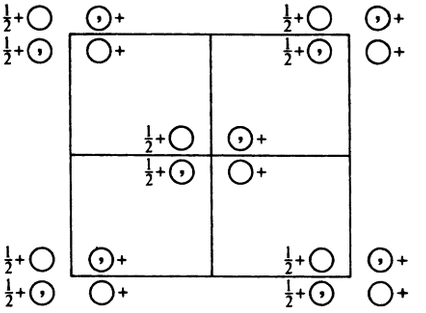
$Cmc2_1$ C_{2v}^{12} $mm2$ Orthorhombic

No. 36 $Cmc2_1$ Patterson symmetry $Cmmm$









Origin on $mc2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) c $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$			Reflection conditions
8 b 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z$	General: hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
4 a m . .	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$			Special: no extra conditions

Symmetry of special projections

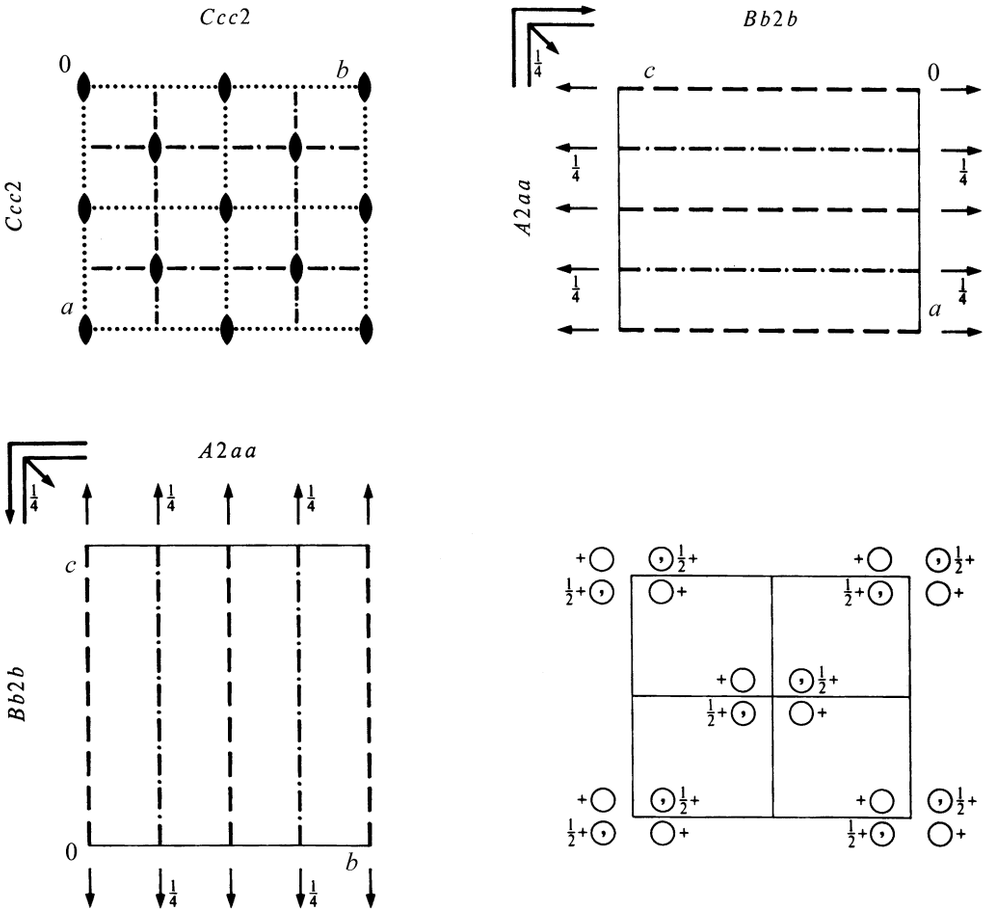
Along [001] $c\,2\,m\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,g\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Ccc2$ C_{2v}^{13} $mm2$ Orthorhombic

No. 37 $Ccc2$ Patterson symmetry $Cmmm$



Origin on $cc2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) c $x,0,z$ (4) c $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z+\frac{1}{2}$	(4) $\bar{x},y,z+\frac{1}{2}$	hkl: $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	c	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$			hkl: $k+l=2n$
4	b	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$			hkl: $l=2n$
4	a	. . 2	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

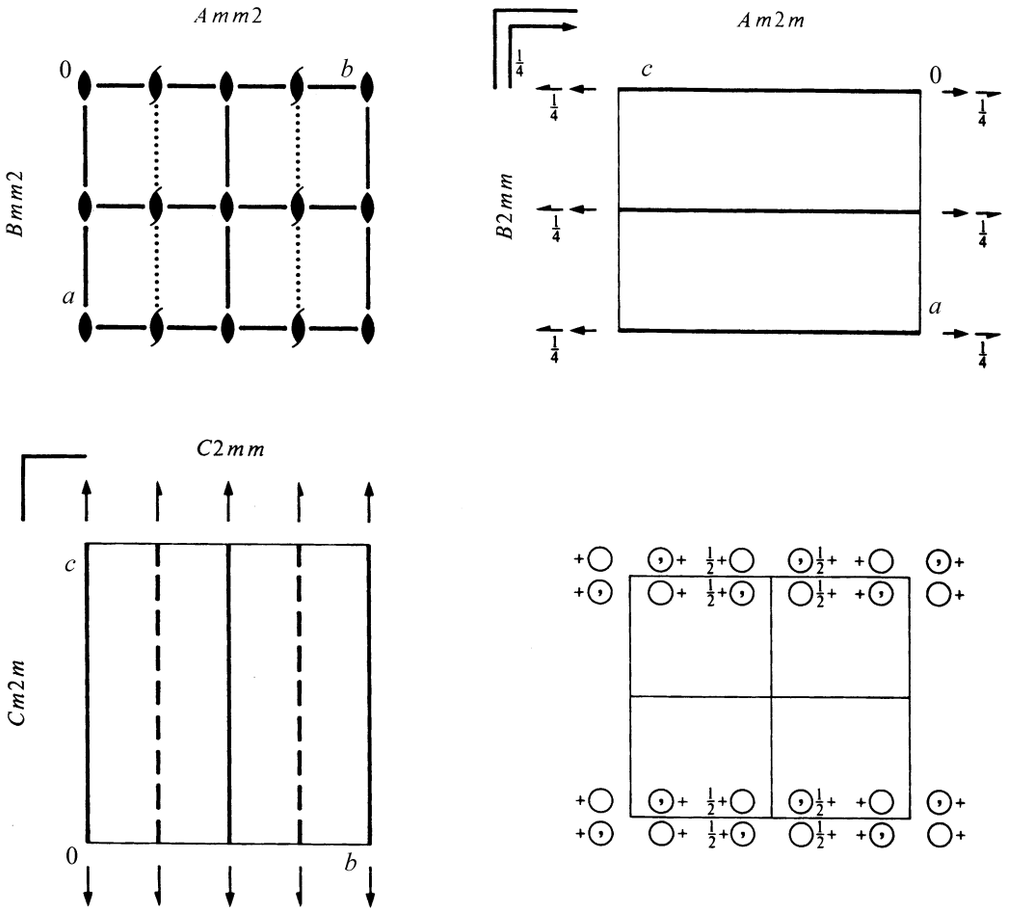
Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

International Tables for Crystallography (2016). Vol. A, Space group 38, pp. 300–301.

$Amm2$ C_{2v}^{14} $mm2$ Orthorhombic

No. 38 $Amm2$

Patterson symmetry $Ammm$ $(Cmmm)$



Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) c $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$			
8	*f*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
4	*e*	*m* . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$		
4	*d*	*m* . .	$0,y,z$	$0,\bar{y},z$		
4	*c*	. *m* .	$x,0,z$	$\bar{x},0,z$		
2	*b*	*m m* 2	$\frac{1}{2},0,z$			
2	*a*	*m m* 2	$0,0,z$			

Reflection conditions

General:

hkl: $k+l=2n$
0*kl*: $k+l=2n$
*h*0*l*: $l=2n$
*hk*0: $k=2n$
0*k*0: $k=2n$
00*l*: $l=2n$

Special: no extra conditions

Symmetry of special projections

Along [001] *p* 2 *m m*
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] *c* 1 *m* 1
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

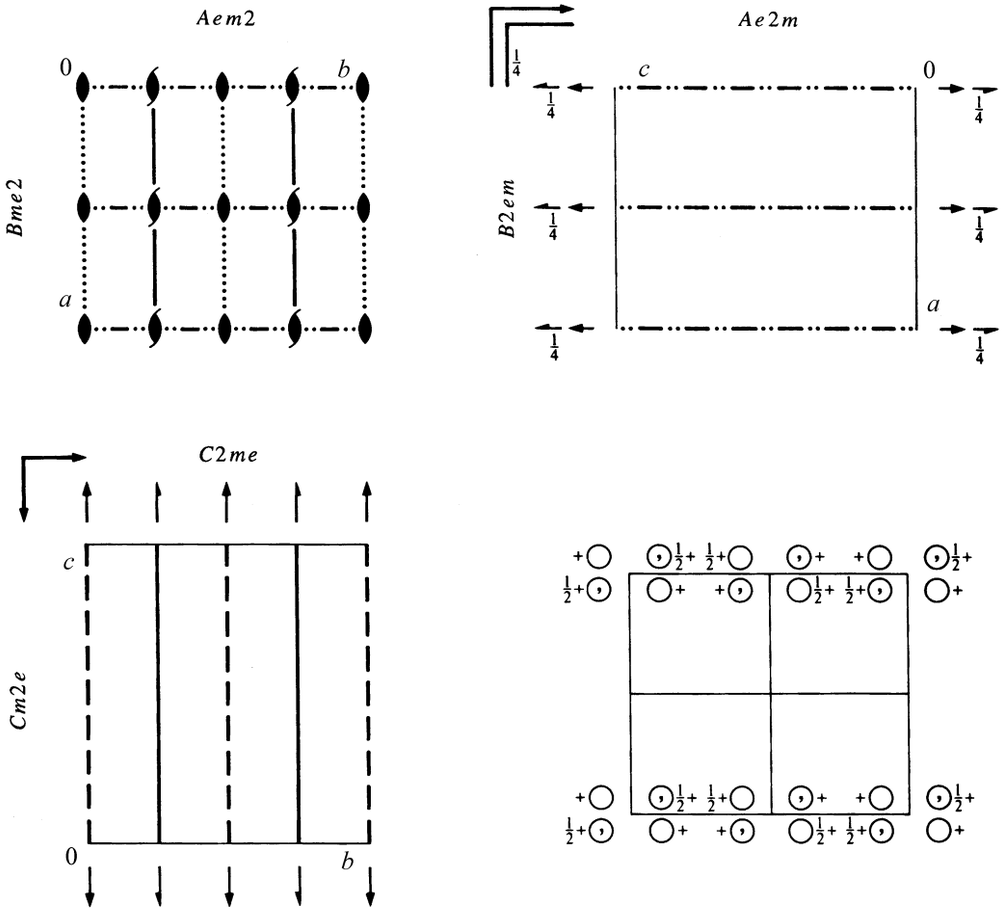
Along [010] *p* 1 1 *m*
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Aem2$ C_{2v}^{15} $mm2$ Orthorhombic

No. 39 $Aem2$

Patterson symmetry $Ammm$ ($Cmmm$)

Former space-group symbol $Abm2$; *cf.* Section 2.1.2



Origin on $ec2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,\frac{1}{4},z$ (4) b $0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) c $x,0,z$ (4) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$			General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y}+\frac{1}{2},z$	(4) $\bar{x},y+\frac{1}{2},z$	hkl: $k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $l=2n$ $hk0$: $k=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	c	. m .	$x,\frac{1}{4},z$	$\bar{x},\frac{3}{4},z$			no extra conditions
4	b	. . 2	$\frac{1}{2},0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl: $k=2n$
4	a	. . 2	$0,0,z$	$0,\frac{1}{2},z$			hkl: $k=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

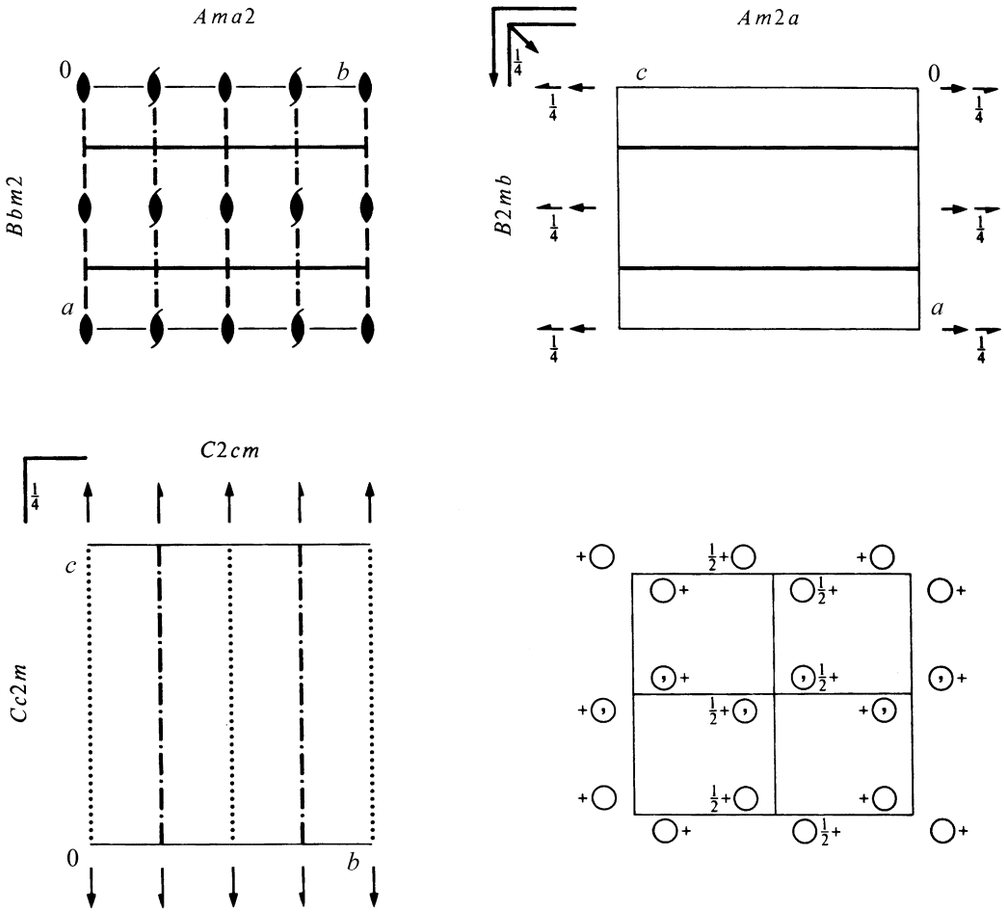
Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Ama2$ C_{2v}^{16} $mm2$ Orthorhombic

No. 40 $Ama2$

Patterson symmetry $Ammm$ ($Cmmm$)



Origin on $1a2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) a $x,0,z$ (4) m $\frac{1}{4},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$			General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	hkl: $k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h,l=2n$ $hk0$: $k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	b	m . .	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			no extra conditions
4	a	. . 2	$0,0,z$	$\frac{1}{2},0,z$			hkl: $h=2n$

Symmetry of special projections

Along [001] $p\,2\,m\,g$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

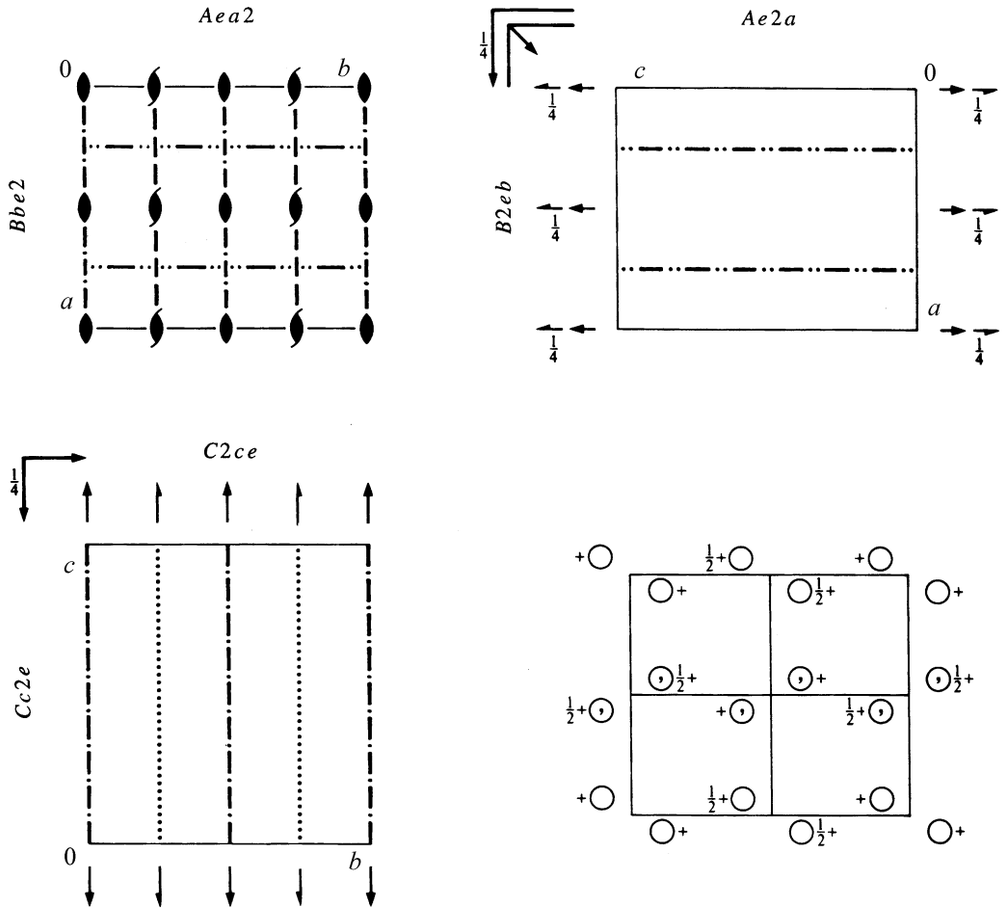
Along [010] $p\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Aea2$ C_{2v}^{17} $mm2$ Orthorhombic

No. 41 $Aea2$

Patterson symmetry $Ammm$ ($Cmmm$)

Former space-group symbol $Aba2$; *cf.* Section 2.1.2



Origin on $1n2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$ (4) c $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$			Reflection conditions
						General:
8	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hkl: $k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
						Special: as above, plus
4	a	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl: $h+k=2n$

Symmetry of special projections

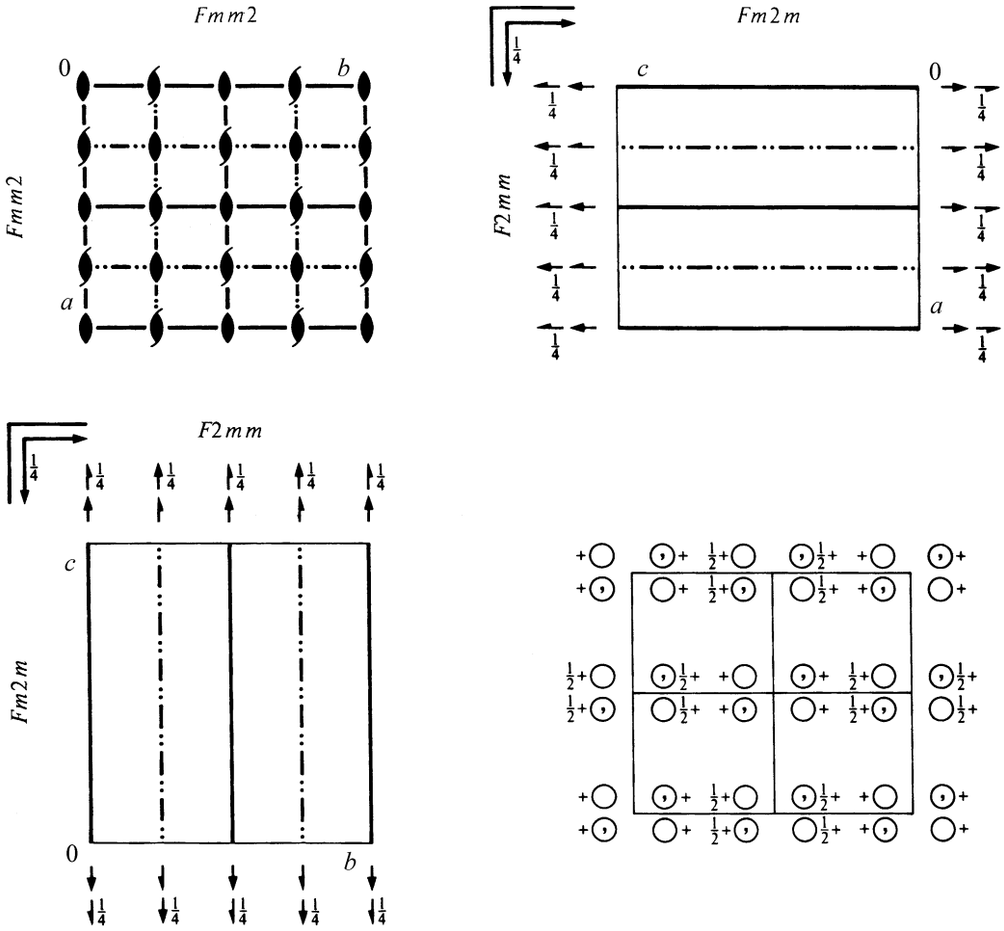
Along [001] $p2mg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Fmm2$ C_{2v}^{18} $mm2$ Orthorhombic

No. 42 $Fmm2$ Patterson symmetry $Fmmm$



Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) c $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$ (4) c $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
				General:
16	e	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $x,\bar{y},z$ (4) $\bar{x},y,z$	hkl: $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
				Special: as above, plus
8	d	$.m.$	$x,0,z$ $\bar{x},0,z$	no extra conditions
8	c	$m..$	$0,y,z$ $0,\bar{y},z$	no extra conditions
8	b	$..2$	$\frac{1}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{3}{4},z$	hkl: $h=2n$
4	a	$mm2$	$0,0,z$	no extra conditions

Symmetry of special projections

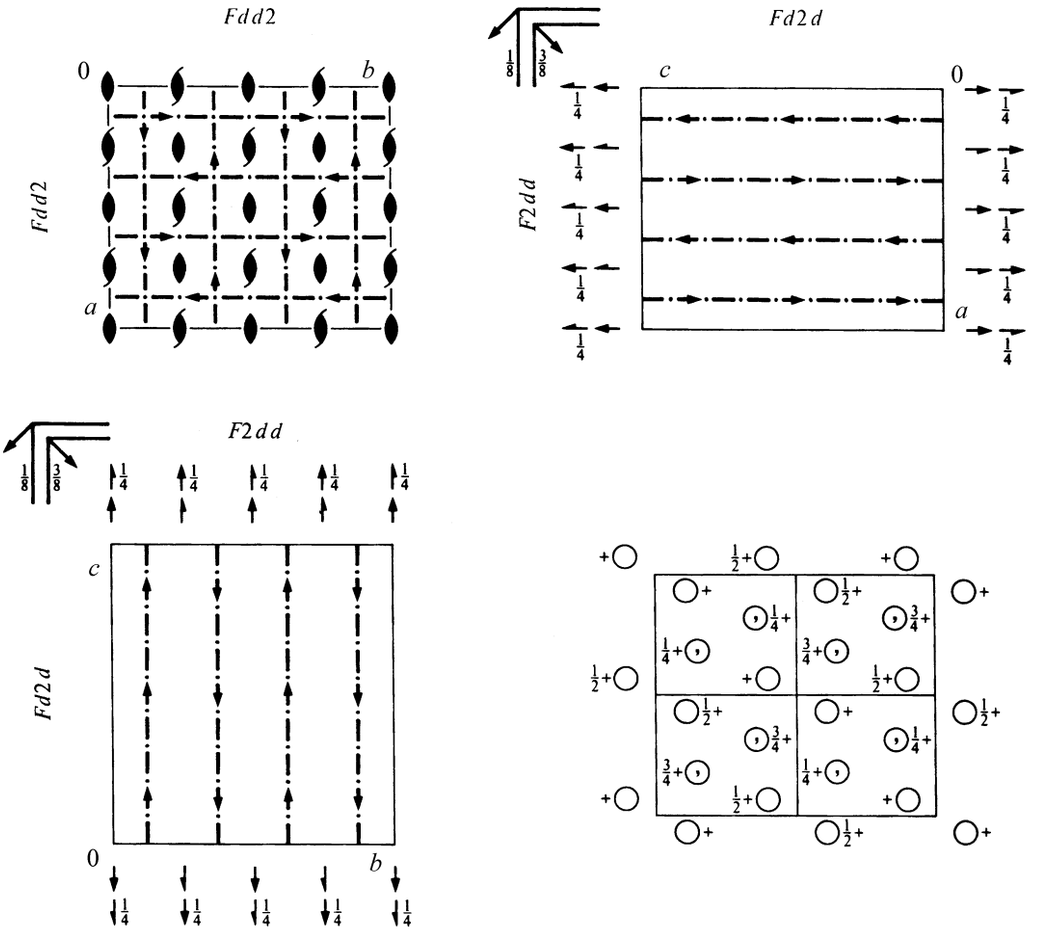
Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Fdd2$ C_{2v}^{19} $mm2$ Orthorhombic

No. 43 $Fdd2$ Patterson symmetry $Fmmm$



Origin on 1 1 2

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) $d(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},z$ (4) $d(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{3}{8},z$ (4) $d(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $d(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},z$ (4) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{3}{8},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{3}{8},z$ (4) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{3}{8},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							General:
16	b	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(4) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$ $0kl$: $k+l=4n$, $k,l=2n$ $h0l$: $h+l=4n$, $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=4n$ $0k0$: $k=4n$ $00l$: $l=4n$
							Special: as above, plus
8	a	. . 2	$0,0,z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{4}$			hkl: $h=2n+1$ or $h+k+l=4n$

Symmetry of special projections

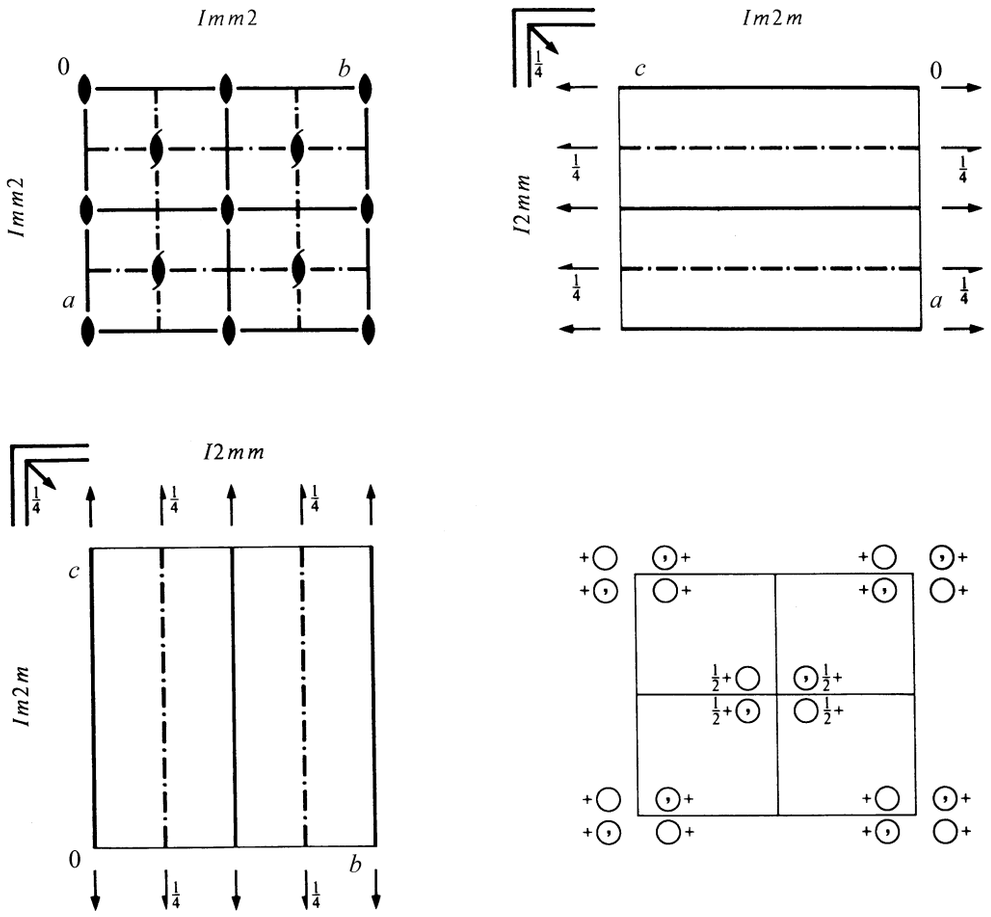
Along [001] $p\,2\,g\,g$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $c\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Imm2$ C_{2v}^{20} $mm2$ Orthorhombic

No. 44 $Imm2$ Patterson symmetry $Immm$



Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$
4	d	m . .	$0,y,z$	$0,\bar{y},z$		
4	c	. m .	$x,0,z$	$\bar{x},0,z$		
2	b	$m\,m\,2$	$0,\frac{1}{2},z$			
2	a	$m\,m\,2$	$0,0,z$			

Reflection conditions

General:

hkl: $h+k+l=2n$
$0kl$: $k+l=2n$
$h0l$: $h+l=2n$
$hk0$: $h+k=2n$
$h00$: $h=2n$
$0k0$: $k=2n$
$00l$: $l=2n$

Special: no extra conditions

Symmetry of special projections

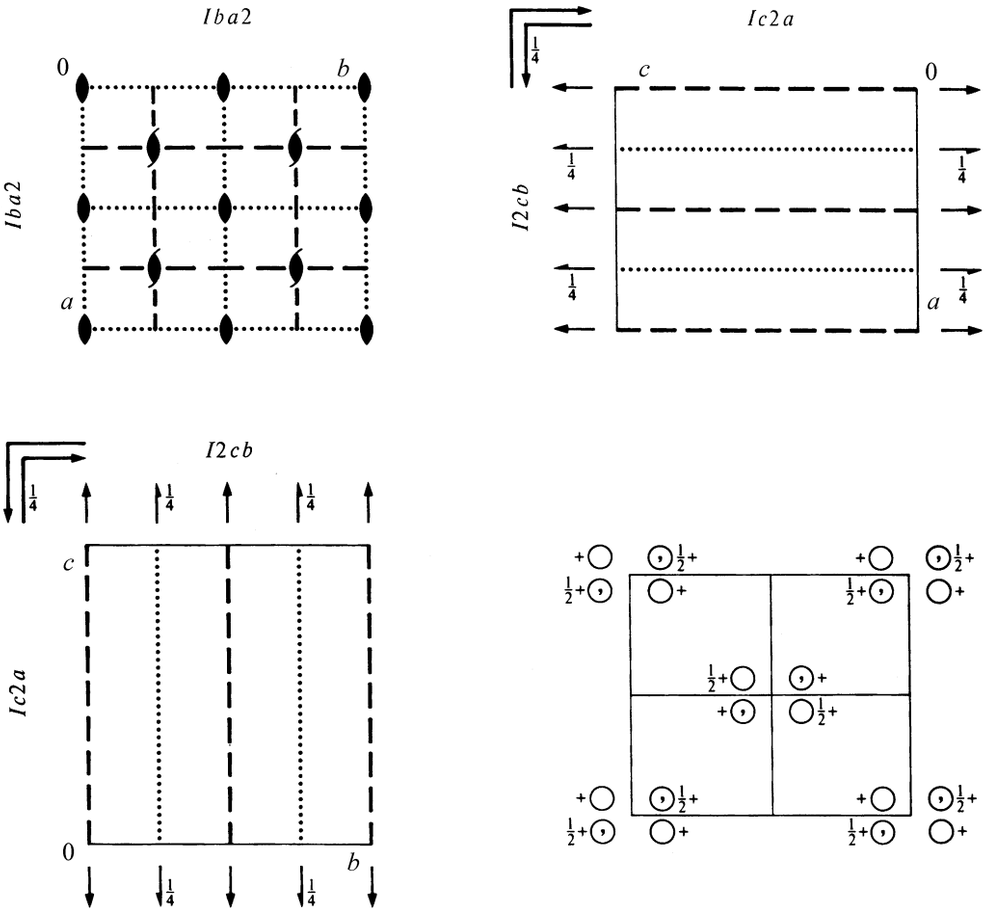
Along [001] $c\,2\,m\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c\,1\,1\,m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Iba2$ C_{2v}^{21} $mm2$ Orthorhombic

No. 45 $Iba2$ Patterson symmetry $Immm$



Origin on $cc2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) c $x,0,z$ (4) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	*c*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	*hkl*: $h+k+l=2n$ 0*kl*: $k,l=2n$ *h*0*l*: $h,l=2n$ *hk*0: $h+k=2n$ *h*00: $h=2n$ 0*k*0: $k=2n$ 00*l*: $l=2n$
							Special: as above, plus
4	*b*	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			*hkl*: $l=2n$
4	*a*	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			*hkl*: $l=2n$

Symmetry of special projections

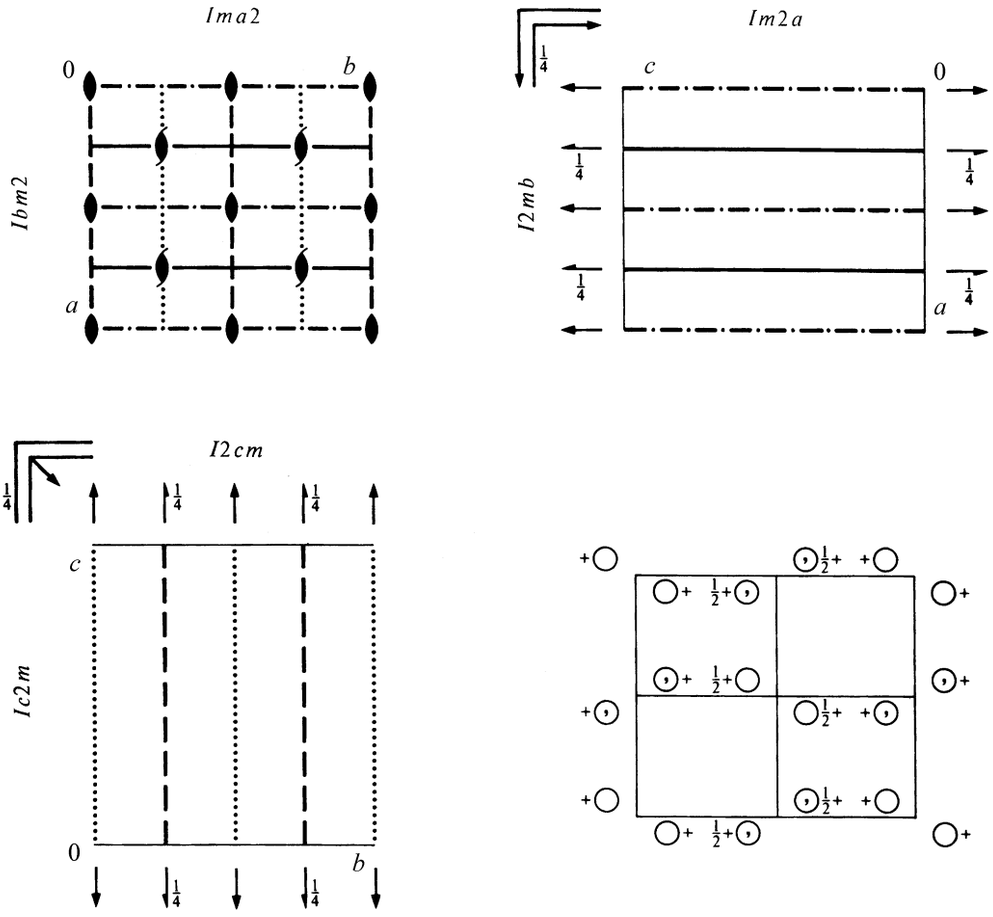
Along [001] *c*2*mm*
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] *p*1*m*1
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] *p*11*m*
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Ima2$ C_{2v}^{22} $mm2$ Orthorhombic

No. 46 $Ima2$ Patterson symmetry $Immm$



Origin on $na2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) a $x,0,z$ (4) m $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) c $x,\frac{1}{4},z$ (4) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
8	*c*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x+\frac{1}{2},\bar{y},z$	(4) $\bar{x}+\frac{1}{2},y,z$	hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*b*	*m* . .	$\frac{1}{4},y,z$	$\frac{3}{4},\bar{y},z$			no extra conditions
4	*a*	. . 2	$0,0,z$	$\frac{1}{2},0,z$			hkl: $h=2n$

Symmetry of special projections

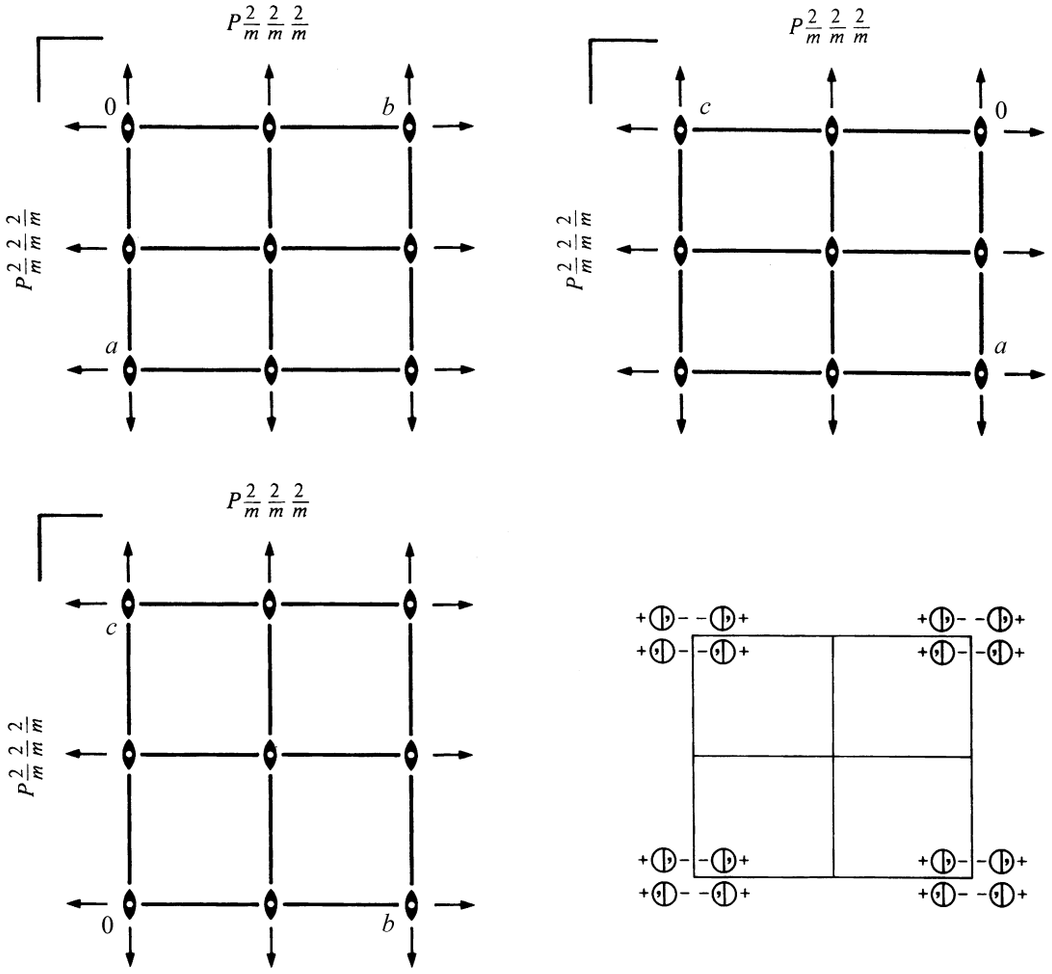
Along [001] $c\,2\,m\,m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p\,1\,1\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Pmmm$ D_{2h}^{1} mmm Orthorhombic

No. 47 $P\ 2/m\ 2/m\ 2/m$ Patterson symmetry $Pmmm$



Origin at centre (mmm)

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) m $x,0,z$	(8) m $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	α	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	no conditions
							Special: no extra conditions
4	z	$..m$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	
4	y	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	
4	x	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$	$x,\frac{1}{2},\bar{z}$	
4	w	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	
4	v	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	
4	u	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	
2	t	$mm2$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	s	$mm2$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	r	$mm2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	q	$mm2$	$0,0,z$	$0,0,\bar{z}$			
2	p	$m2m$	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$			
2	o	$m2m$	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	n	$m2m$	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	m	$m2m$	$0,y,0$	$0,\bar{y},0$			
2	l	$2mm$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$			
2	k	$2mm$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			
2	j	$2mm$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
2	i	$2mm$	$x,0,0$	$\bar{x},0,0$			
1	h	mmm	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	mmm	$0,\frac{1}{2},\frac{1}{2}$				
1	f	mmm	$\frac{1}{2},\frac{1}{2},0$				
1	e	mmm	$0,\frac{1}{2},0$				
1	d	mmm	$\frac{1}{2},0,\frac{1}{2}$				
1	c	mmm	$0,0,\frac{1}{2}$				
1	b	mmm	$\frac{1}{2},0,0$				
1	a	mmm	$0,0,0$				

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

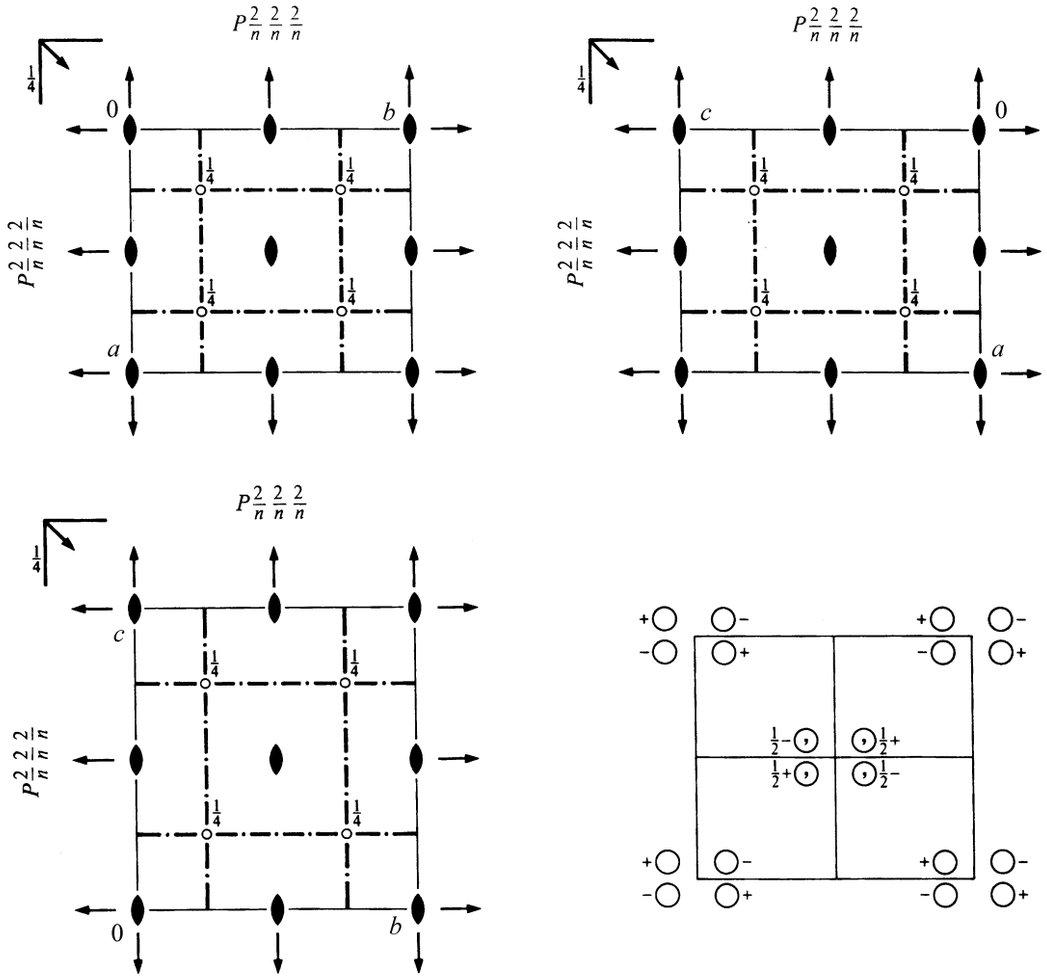
Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

$Pnnn$ D_{2h}^2 *mmm* Orthorhombic

No. 48 $P\ 2/n\ 2/n\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at 222, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*m*	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*l*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	*k*	. . 2	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	*j*	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$	$0,\bar{y}+\frac{1}{2},\frac{1}{2}$	$0,y+\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$
4	*i*	. 2 .	$0,y,0$	$0,\bar{y},0$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$
4	*h*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	hkl: $h+k+l=2n$
4	*g*	2 . .	$x,0,0$	$\bar{x},0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$
4	*f*	$\bar{1}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$
4	*e*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
2	*d*	2 2 2	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	*c*	2 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	*b*	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$
2	*a*	2 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

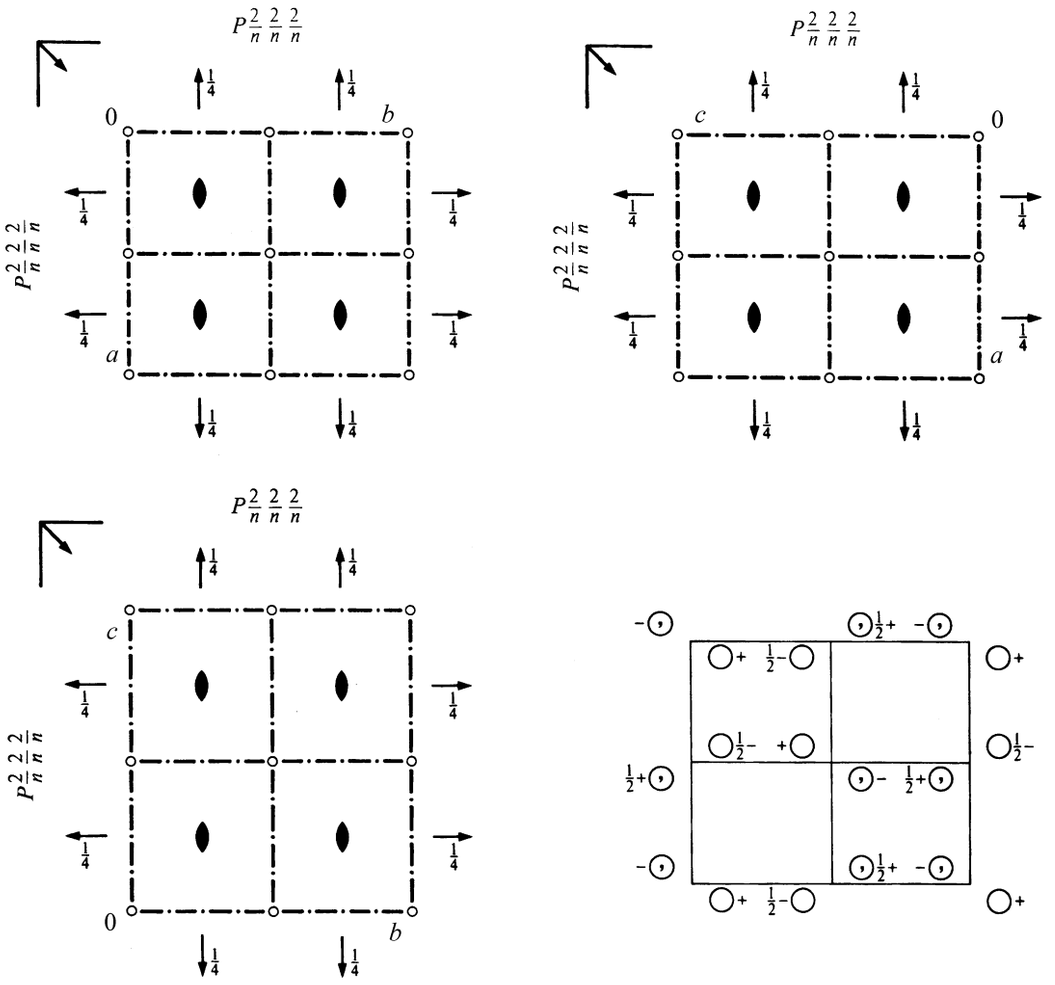
Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Pnnn$ D_{2h}^2 *mmm* Orthorhombic

No. 48 $P\ 2/n\ 2/n\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at nnn, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from 222

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*m*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*l*	. . 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	*k*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	*j*	. 2 .	$\frac{3}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{3}{4}$	hkl: $h+k+l=2n$
4	*i*	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{3}{4},y+\frac{1}{2},\frac{3}{4}$	hkl: $h+k+l=2n$
4	*h*	2 . .	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	hkl: $h+k+l=2n$
4	*g*	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	hkl: $h+k+l=2n$
4	*f*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
4	*e*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl: $h+k,h+l,k+l=2n$
2	*d*	2 2 2	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			hkl: $h+k+l=2n$
2	*c*	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$			hkl: $h+k+l=2n$
2	*b*	2 2 2	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k+l=2n$
2	*a*	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k+l=2n$

Symmetry of special projections

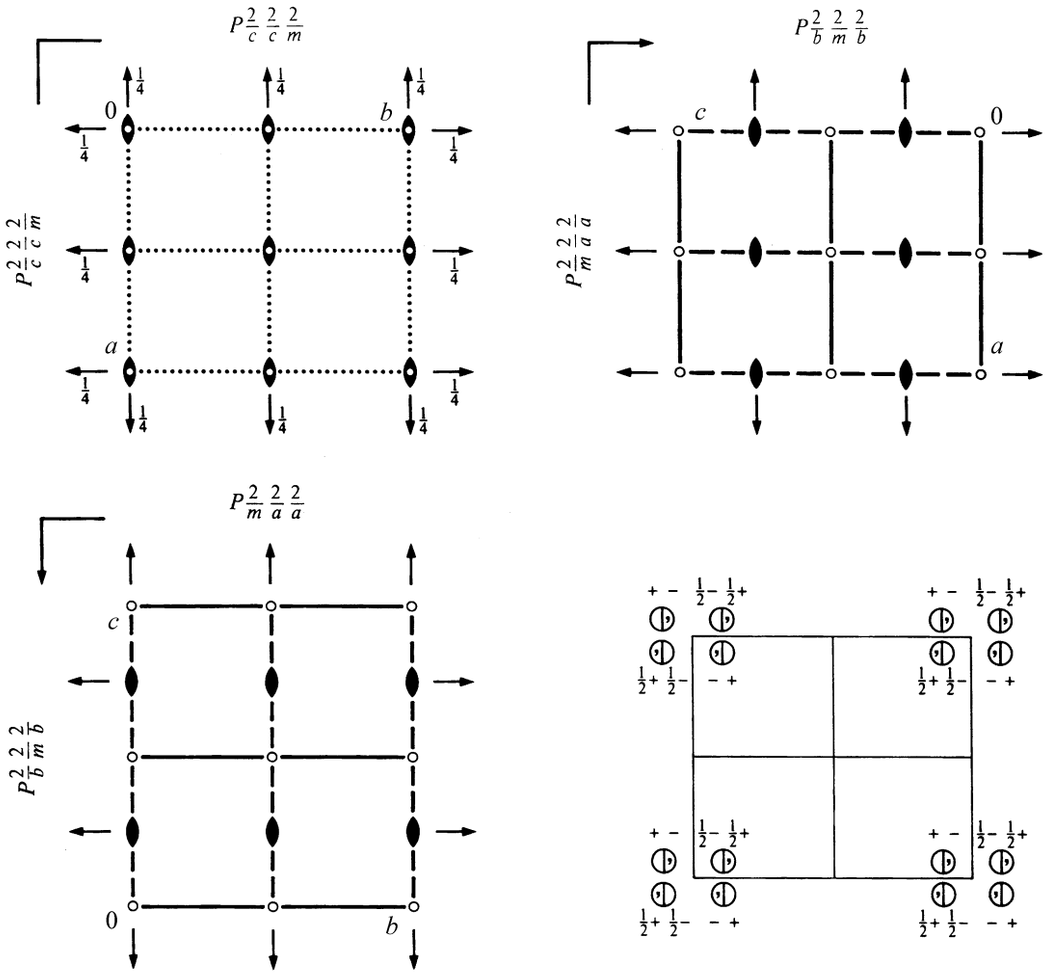
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $\frac{1}{4},y,\frac{1}{4}$

$Pccm$ D_{2h}^3 mmm Orthorhombic

No. 49 $P\ 2/c\ 2/c\ 2/m$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) 2 $x,0,\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) c $x,0,z$	(8) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*r*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*q*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
4	*p*	. . 2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl: $l=2n$
4	*o*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
4	*n*	. . 2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
4	*m*	. . 2	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
4	*l*	. 2 .	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$	hkl: $l=2n$
4	*k*	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
4	*j*	2 . .	$x,\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{3}{4}$	$x,\frac{1}{2},\frac{3}{4}$	hkl: $l=2n$
4	*i*	2 . .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
2	*h*	2 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	*g*	2 2 2	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	*f*	2 2 2	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl: $l=2n$
2	*e*	2 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$
2	*d*	. . 2/*m*	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $l=2n$
2	*c*	. . 2/*m*	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	*b*	. . 2/*m*	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	*a*	. . 2/*m*	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

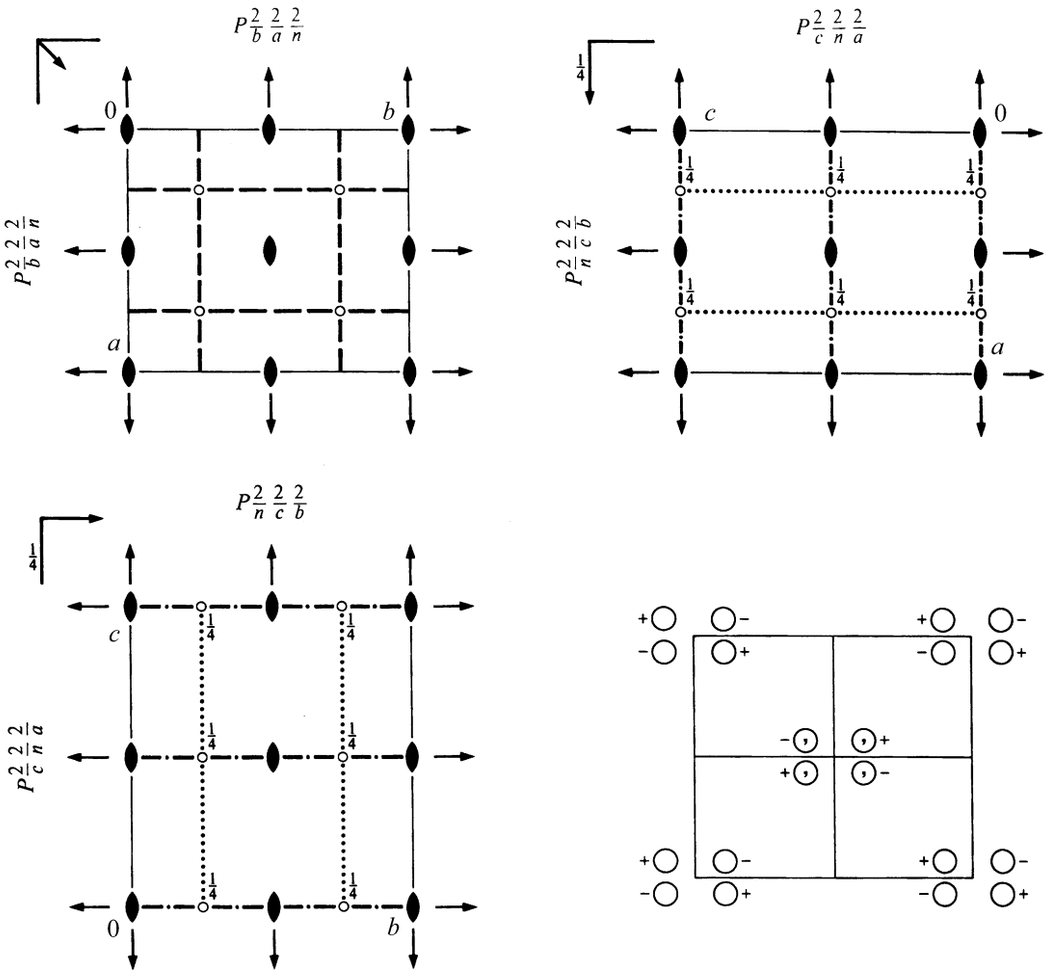
Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

$Pban$ D_{2h}^4 mmm Orthorhombic

No. 50 $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at $222/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) a $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*m*	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*l*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	hkl: $h+k=2n$
4	*k*	. . 2	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl: $h+k=2n$
4	*j*	. 2 .	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
4	*i*	. 2 .	$0,y,0$	$0,\bar{y},0$	$\frac{1}{2},\bar{y}+\frac{1}{2},0$	$\frac{1}{2},y+\frac{1}{2},0$	hkl: $h+k=2n$
4	*h*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
4	*g*	2 . .	$x,0,0$	$\bar{x},0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	hkl: $h+k=2n$
4	*f*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	hkl: $h,k=2n$
4	*e*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hkl: $h,k=2n$
2	*d*	2 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	*c*	2 2 2	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	*b*	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl: $h+k=2n$
2	*a*	2 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

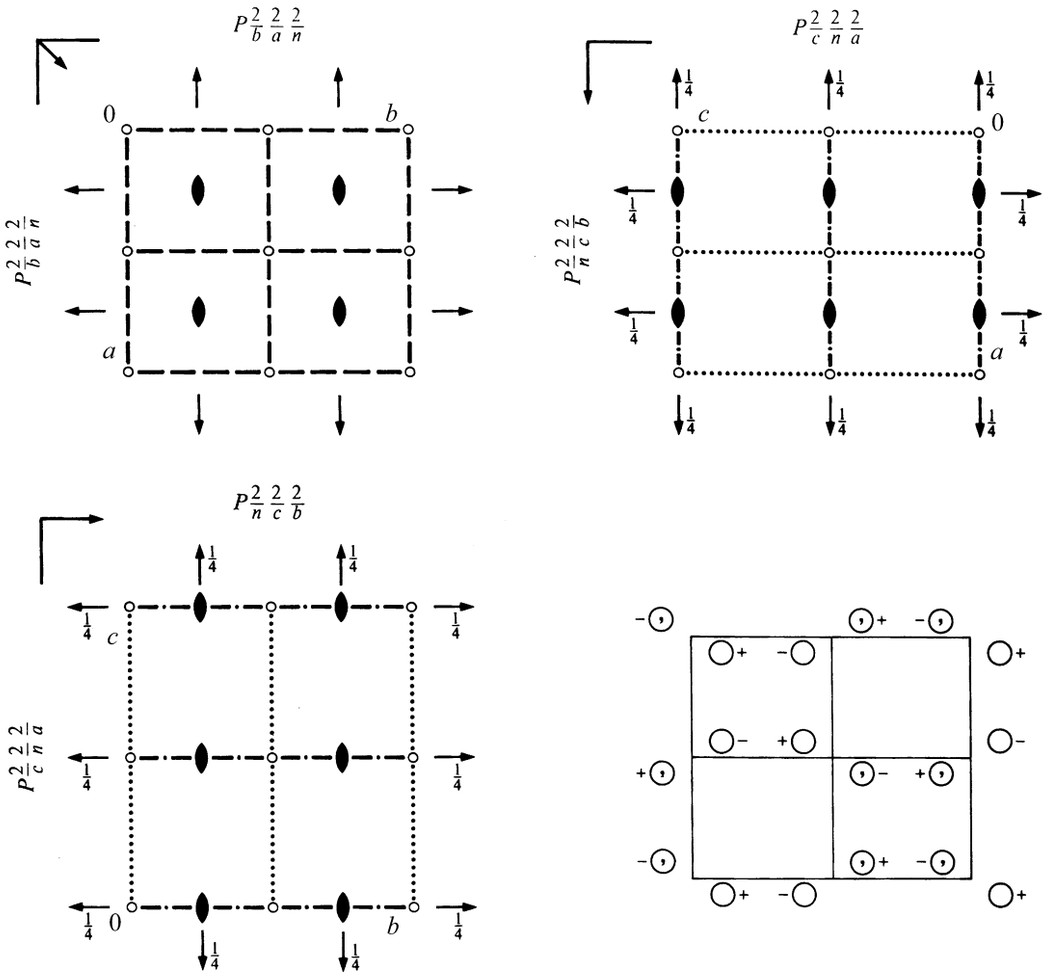
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

Pban D_{2h}^4 *mmm* Orthorhombic

No. 50 $P\ 2/b\ 2/a\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at ban, at $-\frac{1}{4},-\frac{1}{4},0$ from 222

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,0$	(4) 2 $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) a $x,0,z$	(8) b $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*m*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}$ (7) $x+\frac{1}{2},\bar{y},z$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*l*	. . 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z$	hkl: $h+k=2n$
4	*k*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z$	hkl: $h+k=2n$
4	*j*	. 2 .	$\frac{1}{4},y,\frac{1}{2}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},y+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
4	*i*	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y+\frac{1}{2},0$	hkl: $h+k=2n$
4	*h*	2 . .	$x,\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$	$\bar{x},\frac{3}{4},\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$	hkl: $h+k=2n$
4	*g*	2 . .	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	hkl: $h+k=2n$
4	*f*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h,k=2n$
4	*e*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h,k=2n$
2	*d*	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	*c*	2 2 2	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	*b*	2 2 2	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hkl: $h+k=2n$
2	*a*	2 2 2	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$			hkl: $h+k=2n$

Symmetry of special projections

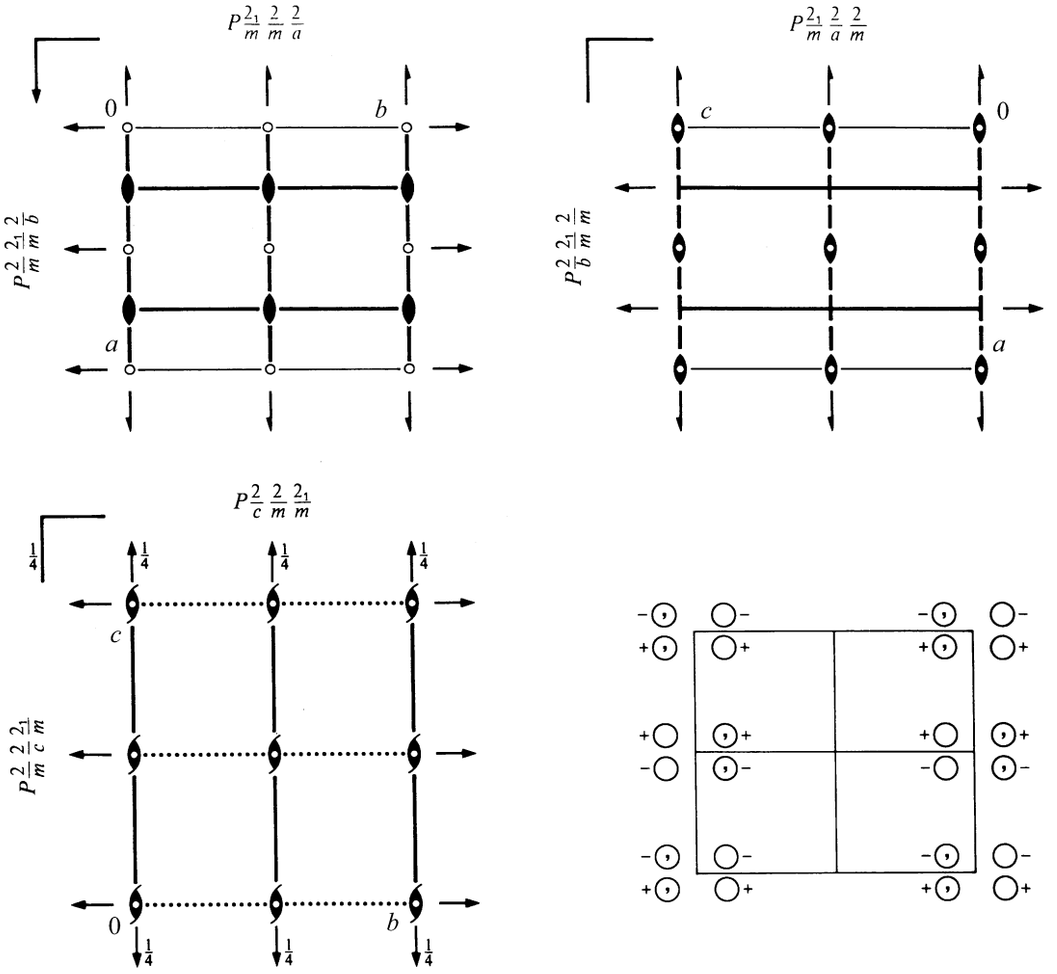
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Pmma$ D_{2h}^5 mmm Orthorhombic

No. 51 $P\ 2_1/m\ 2/m\ 2/a$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$ at $2_1\,2/m\,a$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1
(2) 2 $\frac{1}{4},0,z$
(3) 2 $0,y,0$
(4) $2(\frac{1}{2},0,0)$ $x,0,0$
(5) $\bar{1}$ $0,0,0$
(6) a $x,y,0$
(7) m $x,0,z$
(8) m $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*l*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z$	$hk0$: $h=2n$ $h00$: $h=2n$
							Special: as above, plus
4	*k*	*m* . .	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y},z$	$\frac{3}{4},y,\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	no extra conditions
4	*j*	. *m* .	$x,\frac{1}{2},z$	$\bar{x}+\frac{1}{2},\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\frac{1}{2},\bar{z}$	no extra conditions
4	*i*	. *m* .	$x,0,z$	$\bar{x}+\frac{1}{2},0,z$	$\bar{x},0,\bar{z}$	$x+\frac{1}{2},0,\bar{z}$	no extra conditions
4	*h*	. 2 .	$0,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$	$\frac{1}{2},y,\frac{1}{2}$	hkl: $h=2n$
4	*g*	. 2 .	$0,y,0$	$\frac{1}{2},\bar{y},0$	$0,\bar{y},0$	$\frac{1}{2},y,0$	hkl: $h=2n$
2	*f*	*m m* 2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}$			no extra conditions
2	*e*	*m m* 2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}$			no extra conditions
2	*d*	. 2/*m* .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h=2n$
2	*c*	. 2/*m* .	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h=2n$
2	*b*	. 2/*m* .	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h=2n$
2	*a*	. 2/*m* .	$0,0,0$	$\frac{1}{2},0,0$			hkl: $h=2n$

Symmetry of special projections

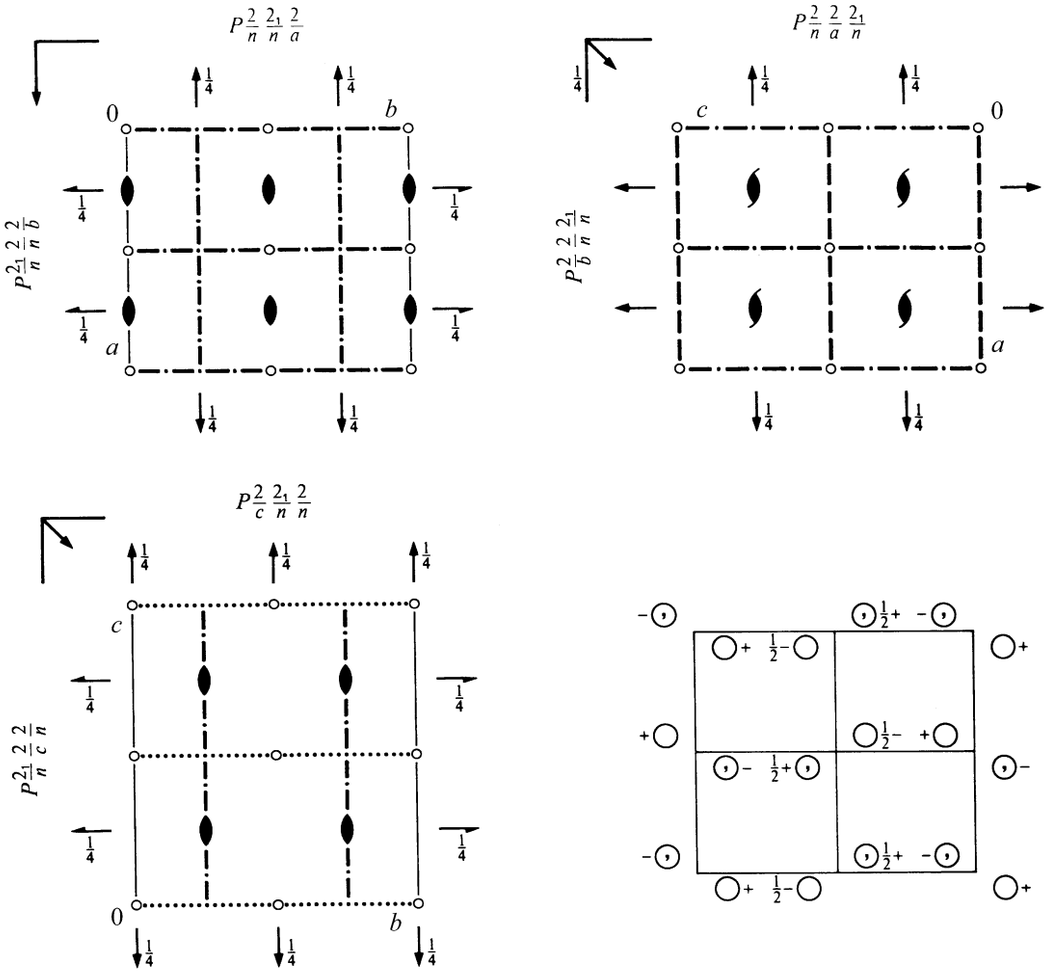
Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

$Pnna$ D_{2h}^{6} mmm Orthorhombic

No. 52 $P\ 2/n\ 2_1/n\ 2/a$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $n\,1\,a$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ 0,0,0	(6) a $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*d*	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	hkl: $h+l=2n$
4	*c*	. . 2	$\frac{1}{4},0,z$	$\frac{1}{4},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{3}{4},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	hkl: $h,k+l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h,k+l=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

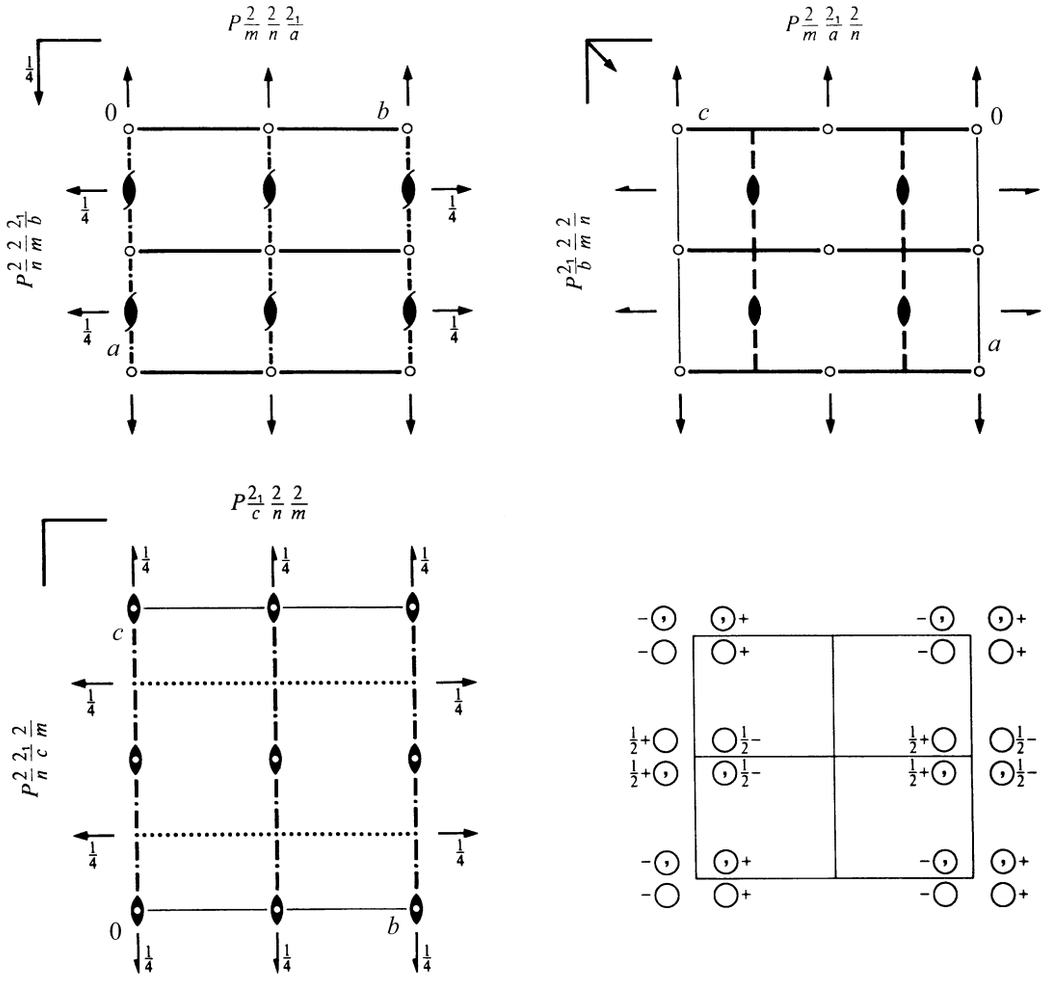
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $\frac{1}{4},y,\frac{1}{4}$

International Tables for Crystallography (2016). Vol. A, Space group 53, pp. 334–335.

$Pmna$ D_{2h}^{7} mmm Orthorhombic

No. 53 $P\ 2/m\ 2/n\ 2_1/a$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$ at $2/mn1$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(8) m $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*i*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	$h0l$: $h+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*h*	*m* . .	$0,y,z$	$\frac{1}{2},\bar{y},z+\frac{1}{2}$	$\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
4	*g*	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{1}{4},\bar{y},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{3}{4},y,\frac{1}{4}$	hkl: $h=2n$
4	*f*	2 . .	$x,\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+l=2n$
4	*e*	2 . .	$x,0,0$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$\bar{x},0,0$	$x+\frac{1}{2},0,\frac{1}{2}$	hkl: $h+l=2n$
2	*d*	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	*c*	$2/m$ . .	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+l=2n$
2	*b*	$2/m$ . .	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$			hkl: $h+l=2n$
2	*a*	$2/m$ . .	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+l=2n$

Symmetry of special projections

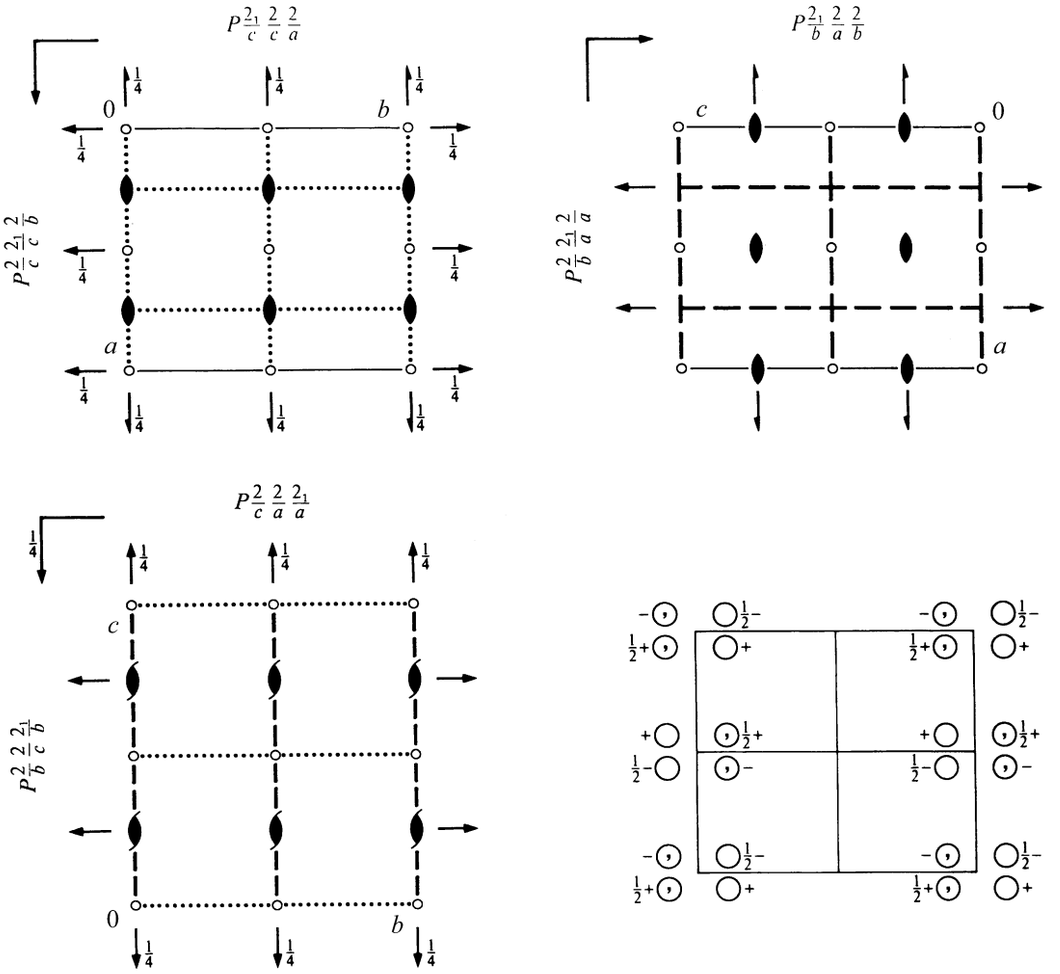
Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

$Pcca$ D_{2h}^{8} mmm Orthorhombic

No. 54 $P\ 2_1/c\ 2/c\ 2/a$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,c\,a$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $\bar{1}$ 0,0,0	(6) a $x,y,0$	(7) c $x,0,z$	(8) c $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*f*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*e*	. . 2	$\frac{1}{4},\frac{1}{2},z$	$\frac{3}{4},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{1}{4},\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
4	*d*	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$	hkl: $l=2n$
4	*c*	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$	hkl: $h+l=2n$
4	*b*	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h,l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h,l=2n$

Symmetry of special projections

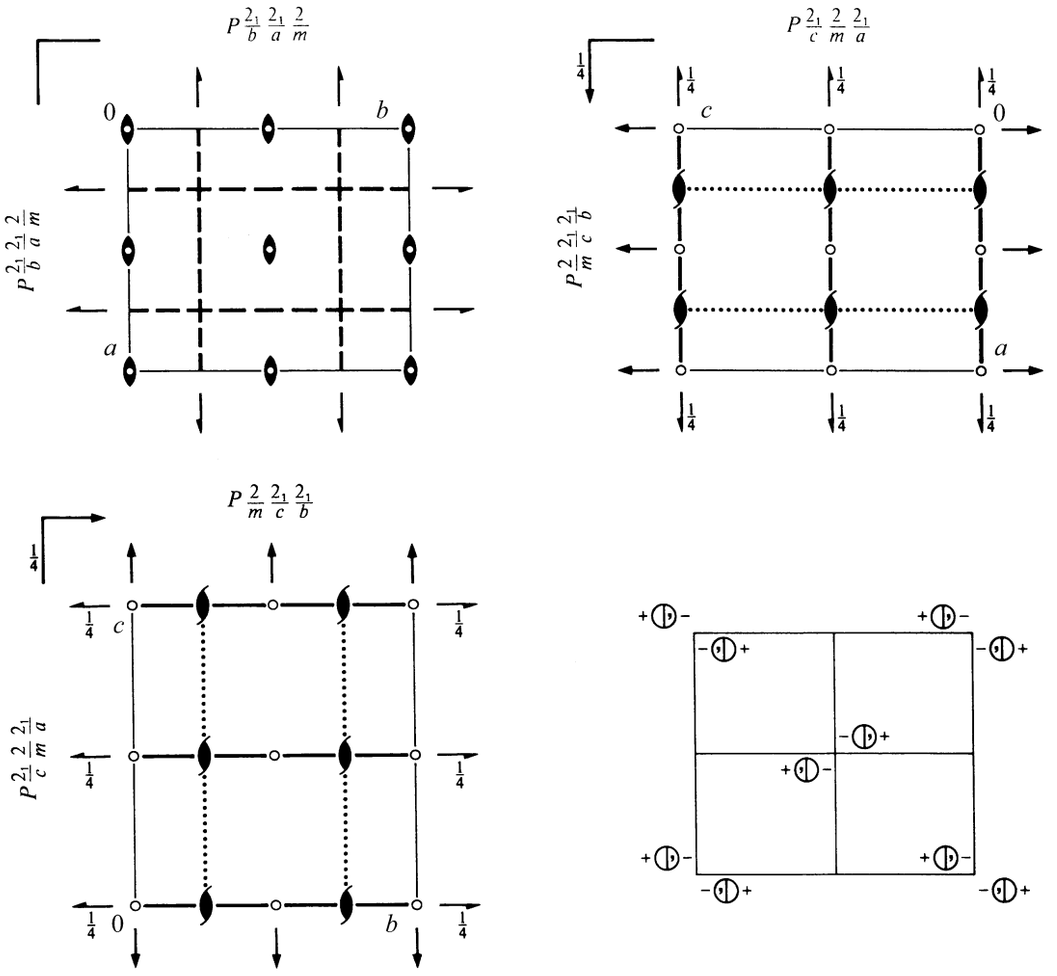
Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Pbam$ D_{2h}^{9} mmm Orthorhombic

No. 55 $P\ 2_1/b\ 2_1/a\ 2/m$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$
(6) m $x,y,0$
(7) a $x,\frac{1}{4},z$
(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*i*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*h*	. . *m*	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	*g*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	no extra conditions
4	*f*	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl: $h+k=2n$
4	*e*	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl: $h+k=2n$
2	*d*	. . 2/*m*	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
2	*c*	. . 2/*m*	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
2	*b*	. . 2/*m*	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	*a*	. . 2/*m*	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

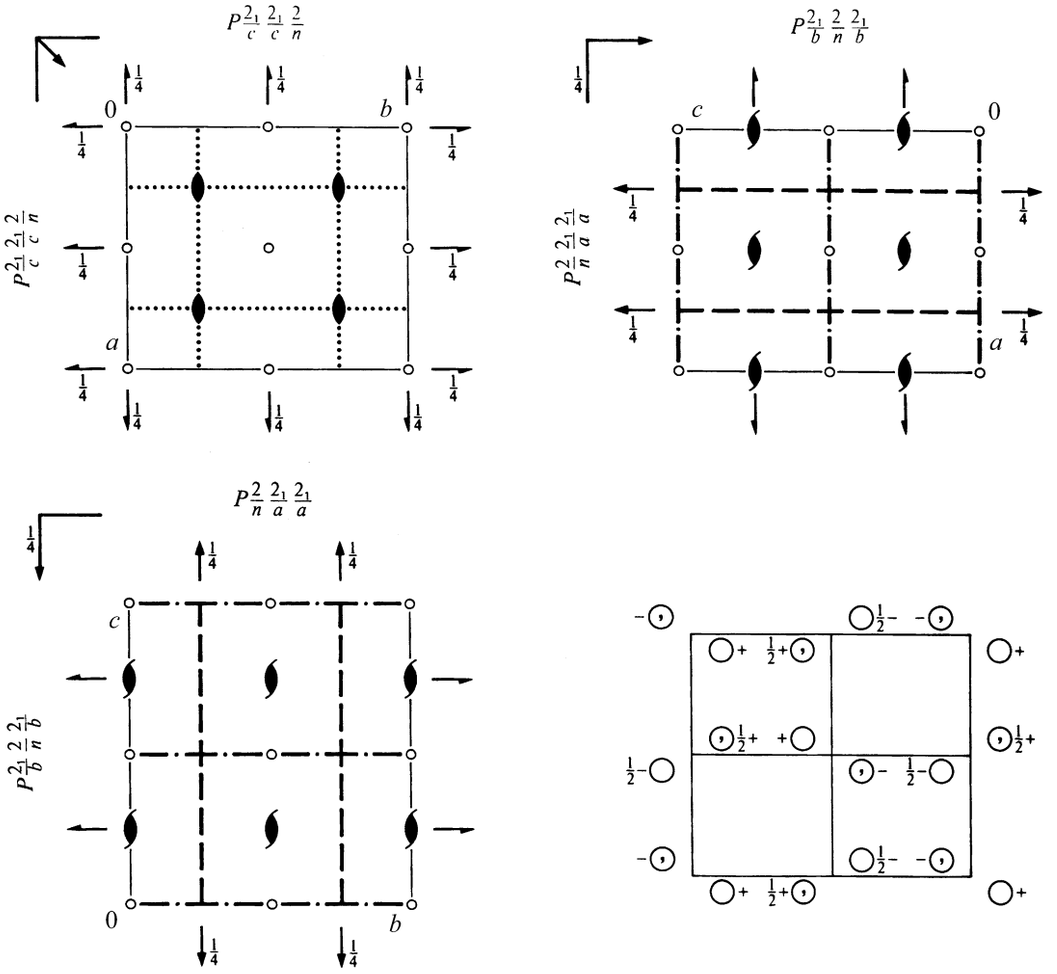
Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Pccn$ D_{2h}^{10} mmm Orthorhombic

No. 56 $P\ 2_1/c\ 2_1/c\ 2/n$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,1\,n$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
(2) $2\ \ \frac{1}{4},\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{4}$
(5) $\bar{1}\ \ 0,0,0$
(6) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$
(7) $c\ \ x,\frac{1}{4},z$
(8) $c\ \ \frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	$0kl$: $l=2n$ $h0l$: $l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*d*	. . 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $l=2n$
4	*c*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	hkl: $l=2n$
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl: $h+k,h+l,k+l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$

Symmetry of special projections

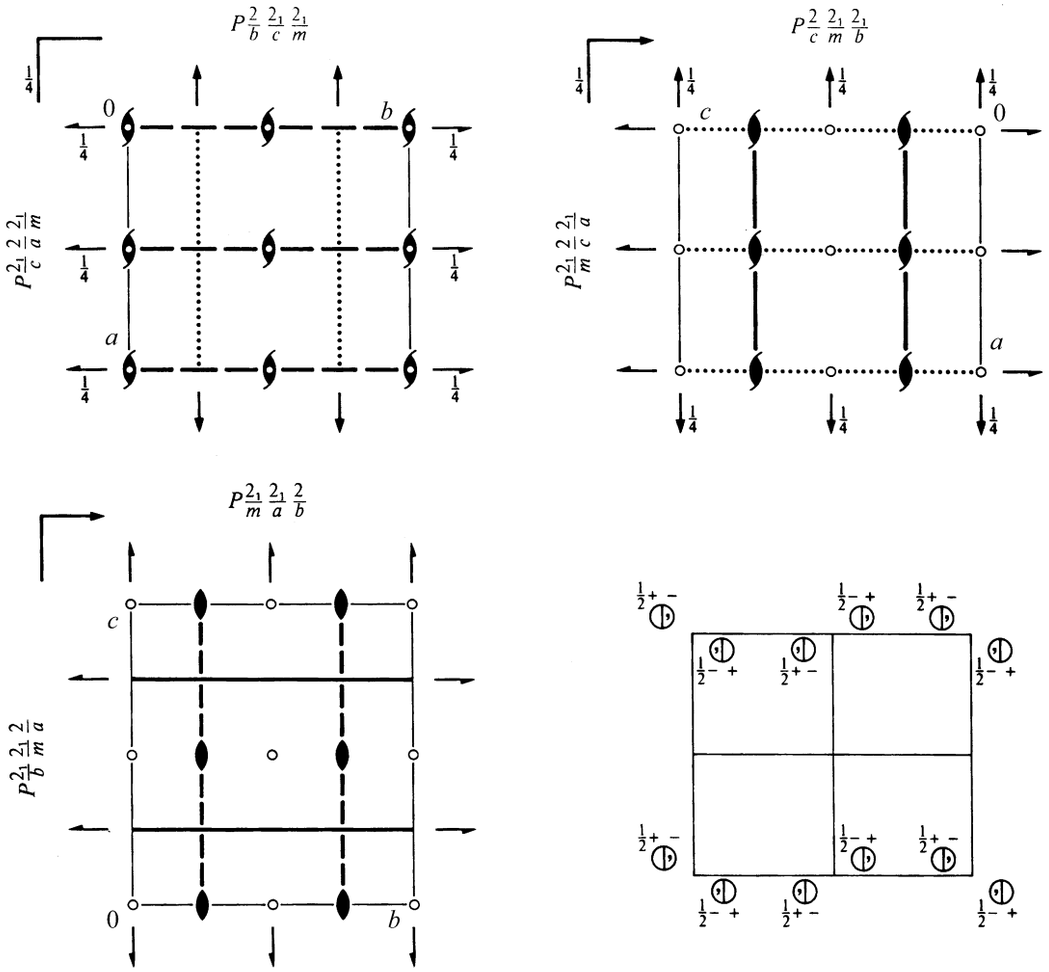
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Pbcm$ D_{2h}^{11} mmm Orthorhombic

No. 57 $P\ 2/b\ 2_1/c\ 2_1/m$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $b\,1\,2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
(2) $2(0,0,\frac{1}{2})$ $0,0,z$
(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$
(4) 2 $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$
(6) m $x,y,\frac{1}{4}$
(7) c $x,\frac{1}{4},z$
(8) b $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*e*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z+\frac{1}{2}$ (6) $x,y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*d*	. . *m*	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$\bar{x},y+\frac{1}{2},\frac{1}{4}$	$x,\bar{y}+\frac{1}{2},\frac{3}{4}$	no extra conditions
4	*c*	2 . .	$x,\frac{1}{4},0$	$\bar{x},\frac{3}{4},\frac{1}{2}$	$\bar{x},\frac{3}{4},0$	$x,\frac{1}{4},\frac{1}{2}$	hkl: $l=2n$
4	*b*	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $k,l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	hkl: $k,l=2n$

Symmetry of special projections

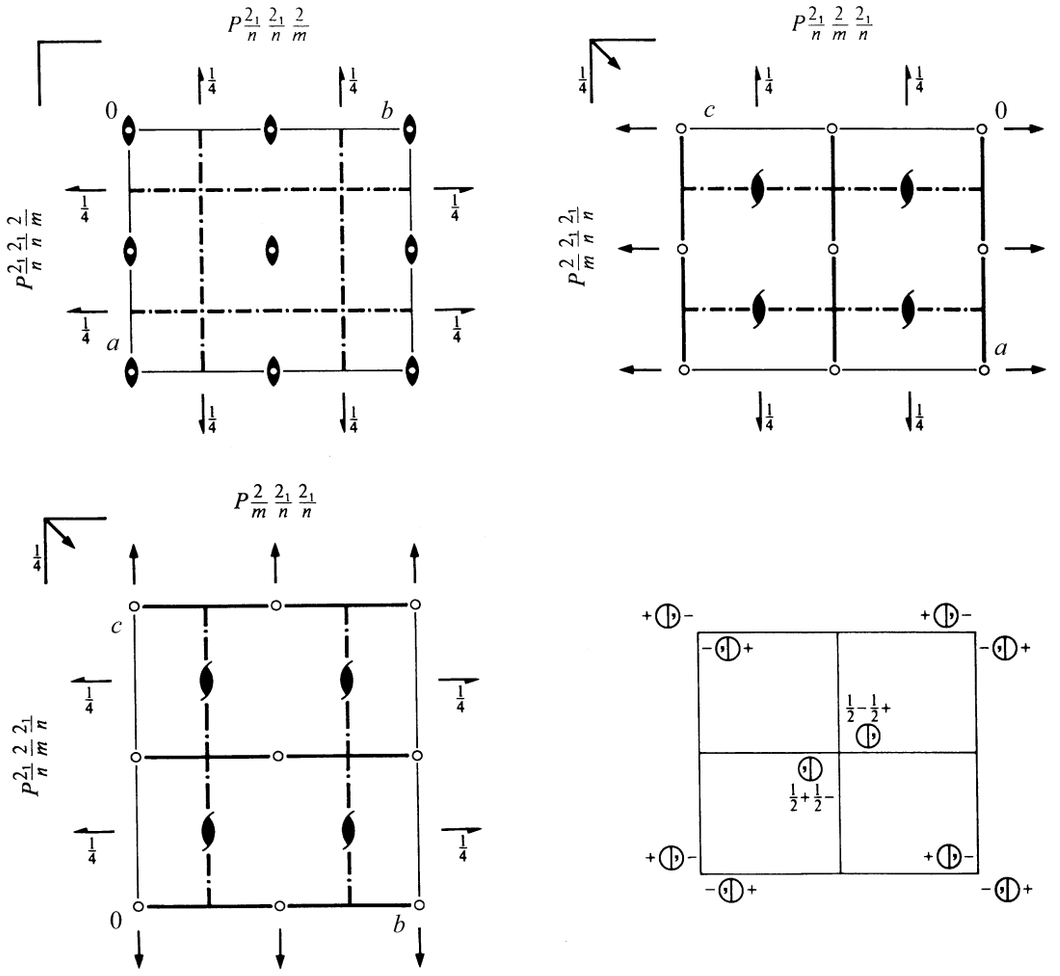
Along [001] $p2gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Pnnm$ D_{2h}^{12} mmm Orthorhombic

No. 58 $P\ 2_1/n\ 2_1/n\ 2/m$ Patterson symmetry $Pmmm$



Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*h*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*g*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	*f*	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	*e*	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k+l=2n$
2	*d*	. . 2/*m*	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl: $h+k+l=2n$
2	*c*	. . 2/*m*	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	*b*	. . 2/*m*	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	*a*	. . 2/*m*	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

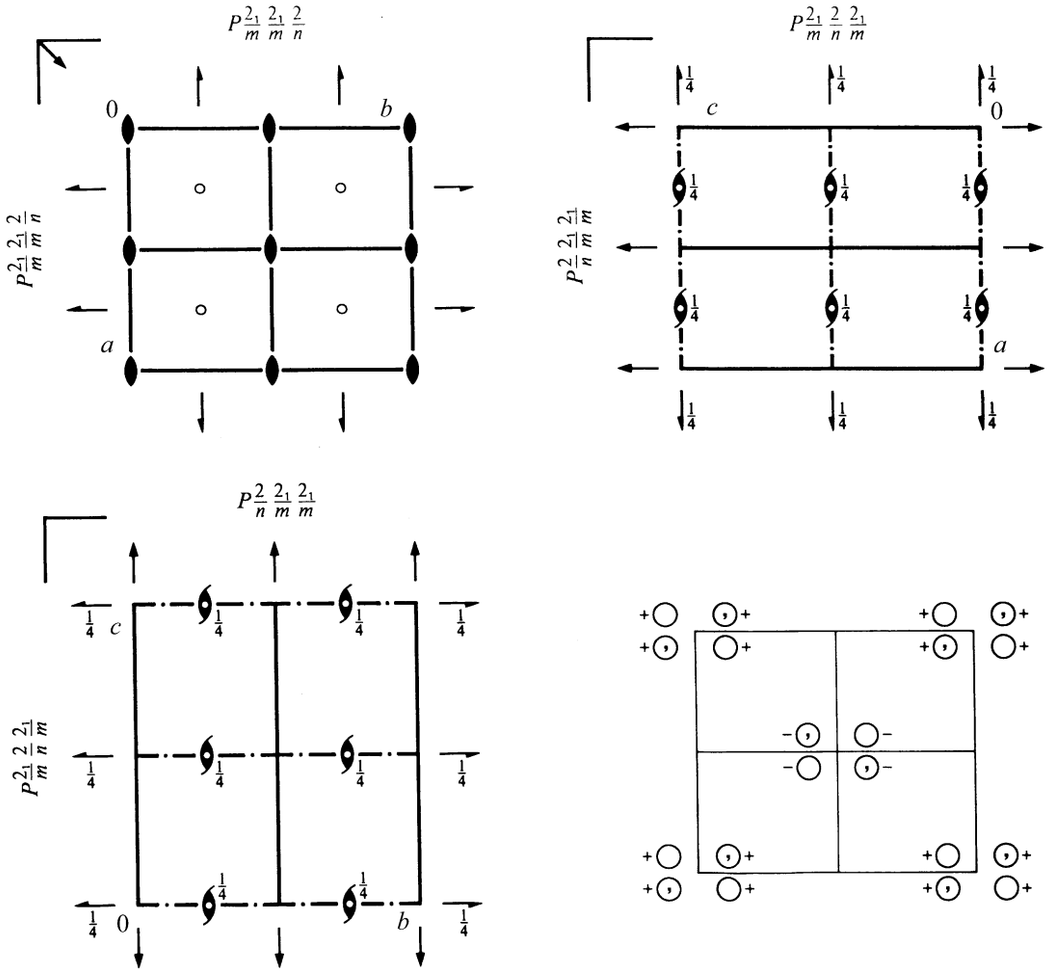
Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Pmmn$ D_{2h}^{13} mmm Orthorhombic

No. 59 $P\ 2_1/m\ 2_1/m\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 1



Origin at $mm2/n$, at $\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) $2\ \ 0,0,z$ (3) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$
(5) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},0$ (6) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$ (7) $m\ \ x,0,z$ (8) $m\ \ 0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*g*	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x},y,z$	$hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*f*	. *m* .	$x,0,z$	$\bar{x},0,z$	$\bar{x}+\frac{1}{2},\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\frac{1}{2},\bar{z}$	no extra conditions
4	*e*	*m* . .	$0,y,z$	$0,\bar{y},z$	$\frac{1}{2},y+\frac{1}{2},\bar{z}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	no extra conditions
4	*d*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl: $h,k=2n$
4	*c*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h,k=2n$
2	*b*	*m m* 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	*a*	*m m* 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

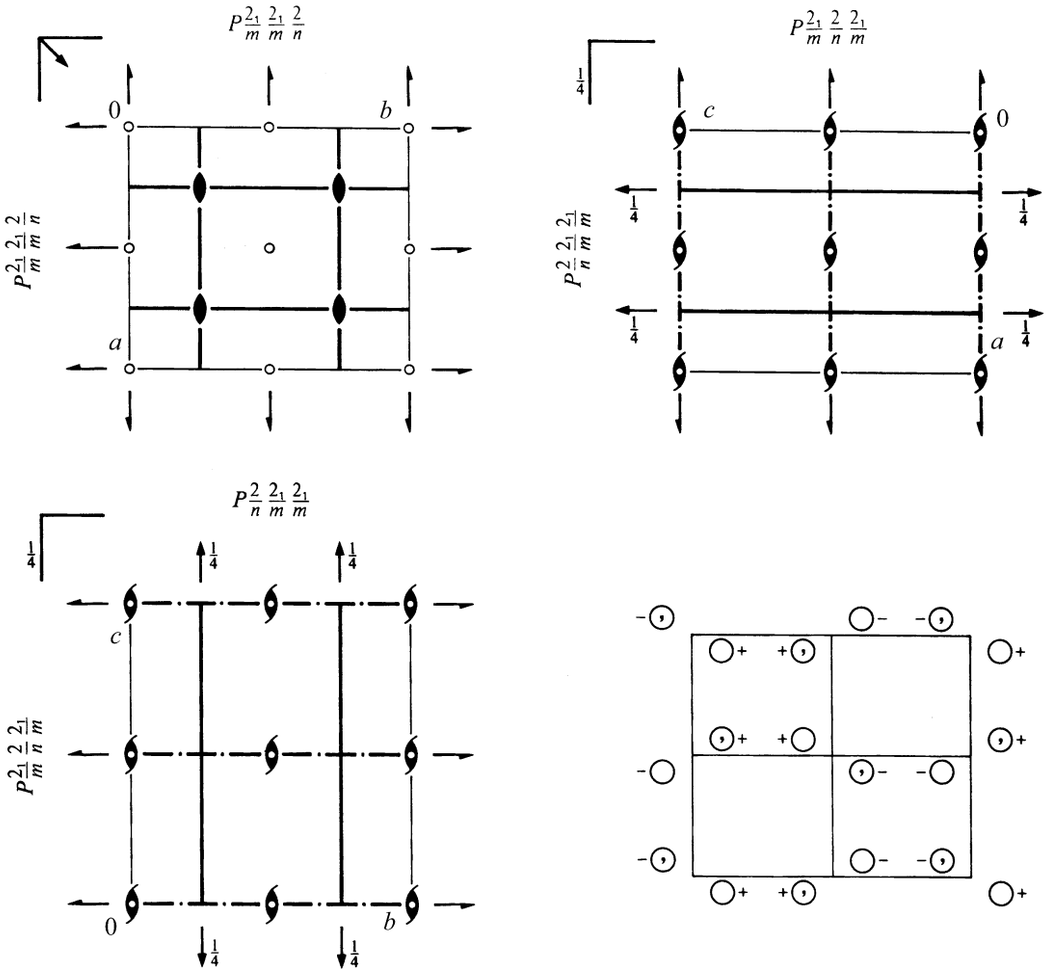
Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [010] $p2gm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $\frac{1}{4},y,0$

$Pmmn$ D_{2h}^{13} mmm Orthorhombic

No. 59 $P\ 2_1/m\ 2_1/m\ 2/n$ Patterson symmetry $Pmmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $2_1 2_1 n$, at $-\frac{1}{4}, -\frac{1}{4}, 0$ from $mm2$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4}, \frac{1}{4}, z$	(3) $2(0, \frac{1}{2}, 0)\ \ 0, y, 0$	(4) $2(\frac{1}{2}, 0, 0)\ \ x, 0, 0$
(5) $\bar{1}\ \ 0, 0, 0$	(6) $n(\frac{1}{2}, \frac{1}{2}, 0)\ \ x, y, 0$	(7) $m\ \ x, \frac{1}{4}, z$	(8) $m\ \ \frac{1}{4}, y, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*g*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z$	$hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*f*	. *m* .	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{3}{4},\bar{z}$	no extra conditions
4	*e*	*m* . .	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$	$\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	no extra conditions
4	*d*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h,k=2n$
4	*c*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl: $h,k=2n$
2	*b*	*m m* 2	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$			no extra conditions
2	*a*	*m m* 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

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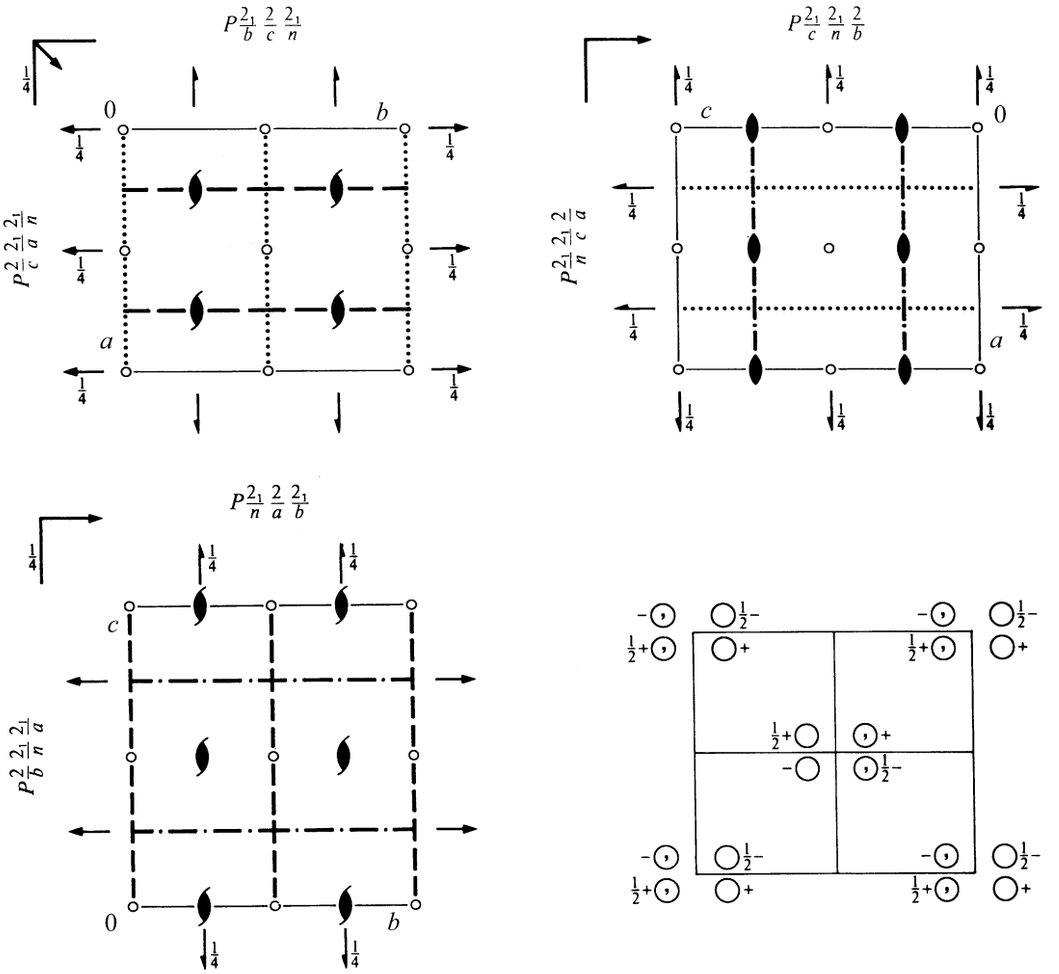
$Pbcn$ D_{2h}^{14} mmm Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,c\,1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) 2 $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) c $x,0,z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*d*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*c*	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{3}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{4}$	hkl: $h+k=2n$
4	*b*	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	hkl: $h+k,l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+k,l=2n$

Symmetry of special projections

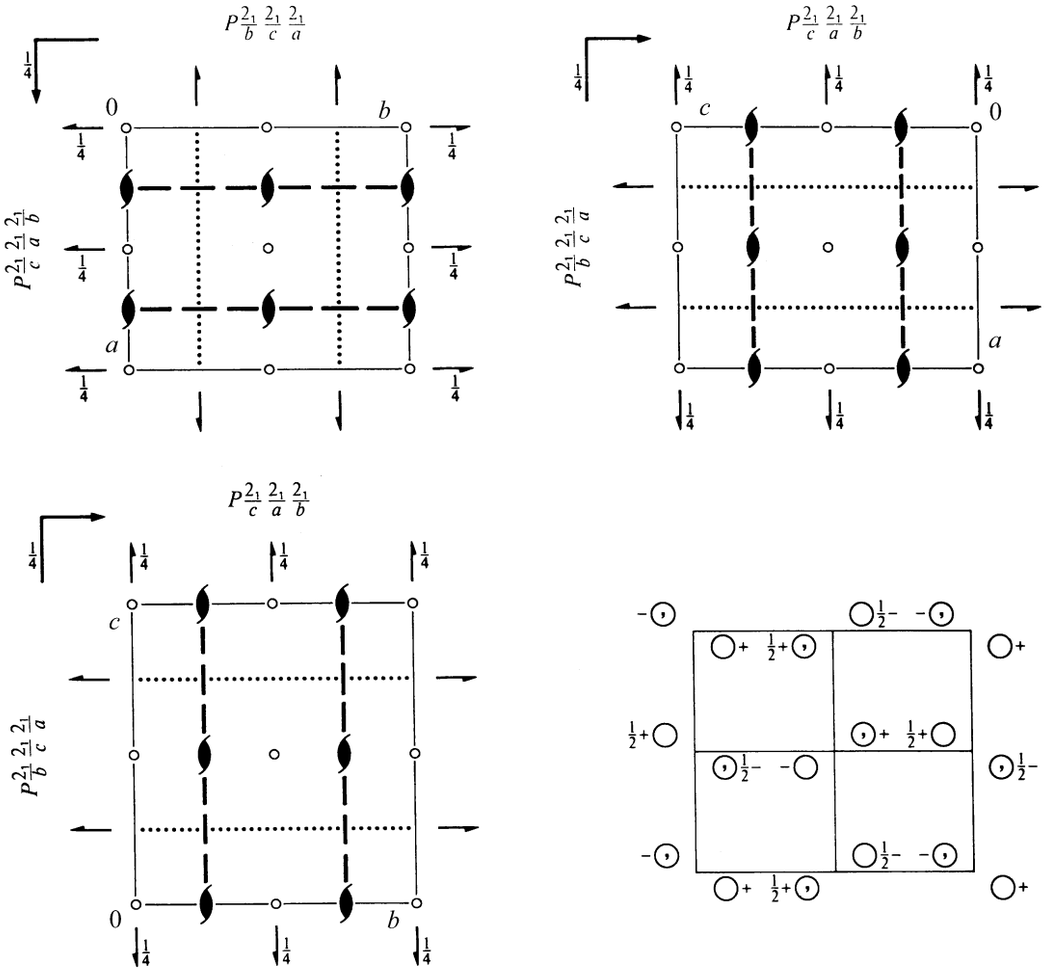
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Pbca$ D_{2h}^{15} mmm Orthorhombic

No. 61 $P\ 2_1/b\ 2_1/c\ 2_1/a$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) c $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*c*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$0kl$: $k=2n$ $h0l$: $l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+k,h+l,k+l=2n$

Symmetry of special projections

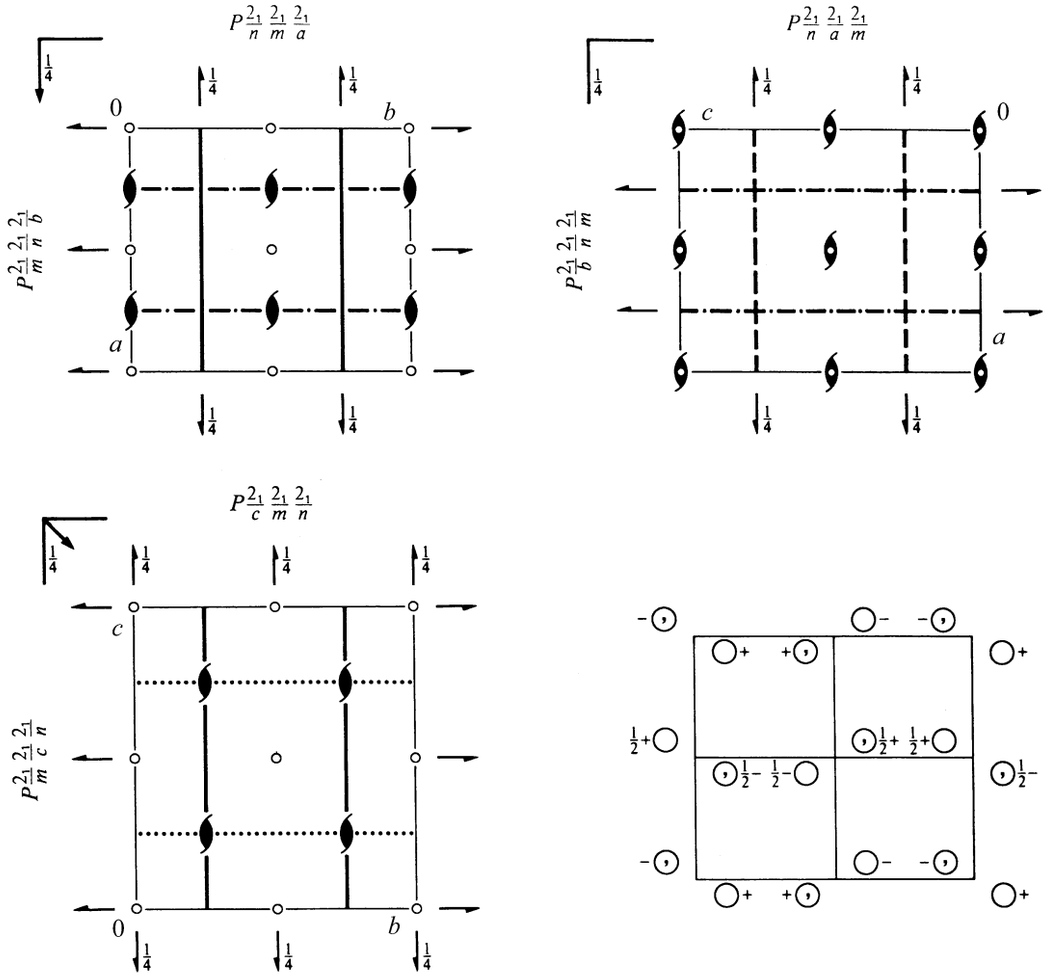
Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Pnma$ D_{2h}^{16} mmm Orthorhombic

No. 62 $P\ 2_1/n\ 2_1/m\ 2_1/a$ Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,2_1\,1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) m $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	*d*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	*c*	. *m* .	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+l,k=2n$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+l,k=2n$

Symmetry of special projections

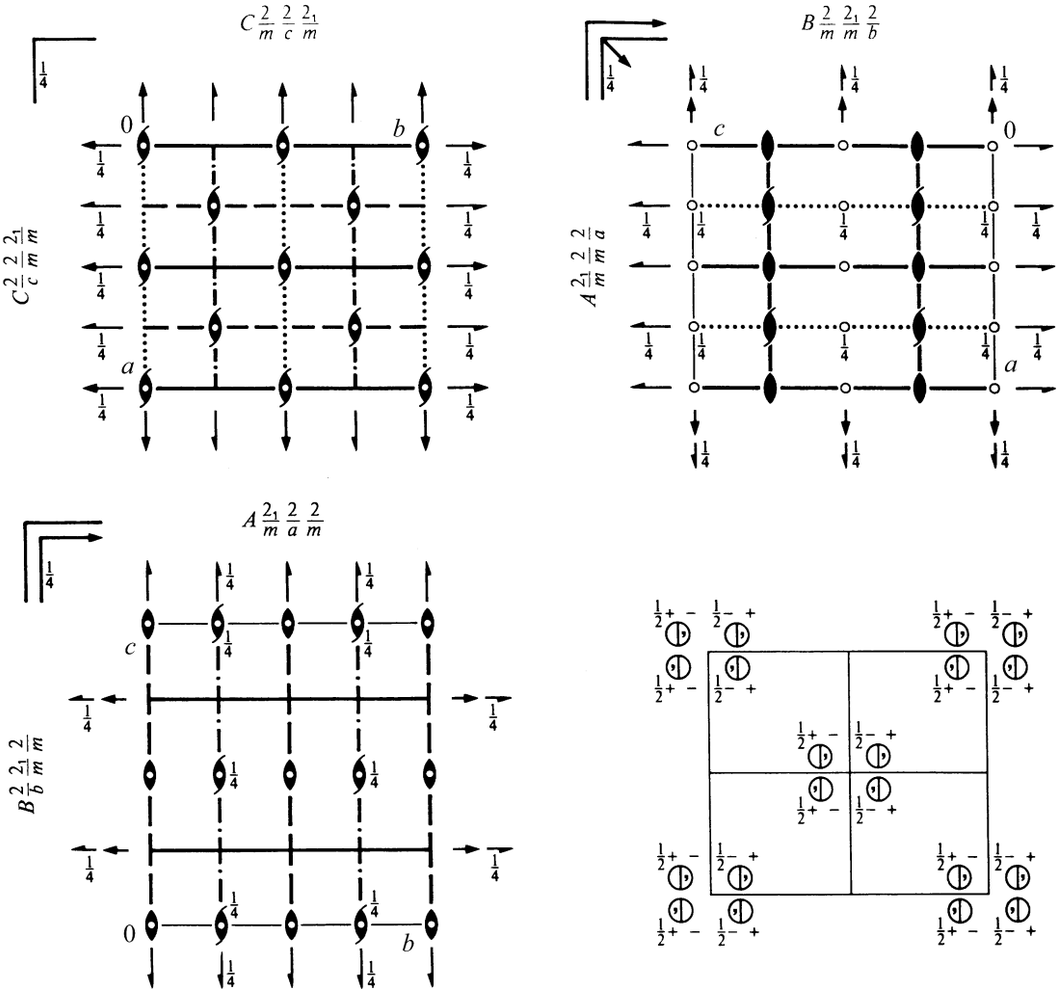
Along [001] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $p2gg$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

$Cmcm$ D_{2h}^{17} mmm Orthorhombic

No. 63 $C\ 2/m\ 2/c\ 2_1/m$ Patterson symmetry $Cmmm$



Origin at centre $(2/m)$ at $2/mc2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $0,0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,\frac{1}{4}$	(7) c $x,0,z$	(8) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	*h*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z+\frac{1}{2}$ (6) $x,y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*g*	. . *m*	$x,y,\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$\bar{x},y,\frac{1}{4}$	$x,\bar{y},\frac{3}{4}$	no extra conditions
8	*f*	*m* . .	$0,y,z$	$0,\bar{y},z+\frac{1}{2}$	$0,y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*e*	2 . .	$x,0,0$	$\bar{x},0,\frac{1}{2}$	$\bar{x},0,0$	$x,0,\frac{1}{2}$	hkl: $l=2n$
8	*d*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	hkl: $k,l=2n$
4	*c*	*m* 2 *m*	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$			no extra conditions
4	*b*	2/*m* . .	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	*a*	2/*m* . .	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

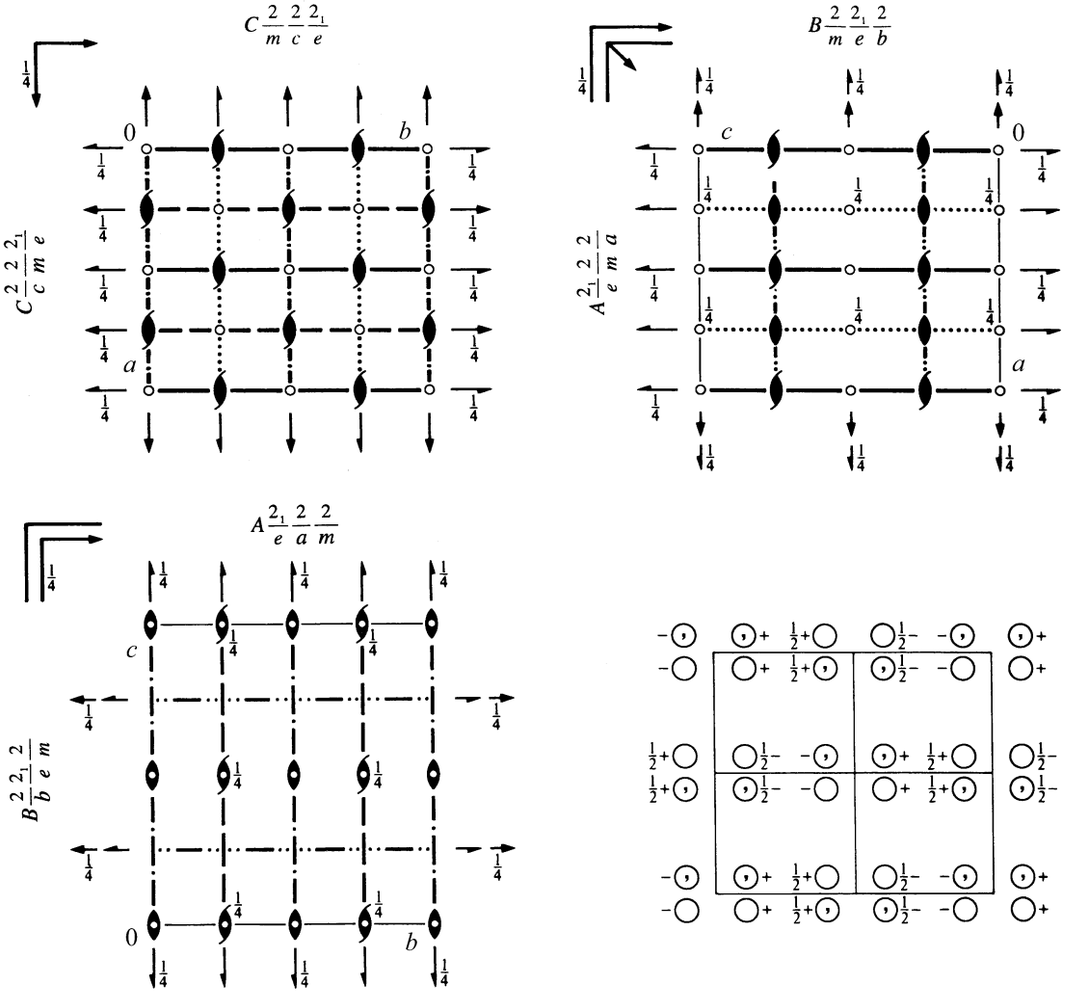
Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

International Tables for Crystallography (2016). Vol. A, Space group 64, pp. 358–359.

$Cmce$ D_{2h}^{18} mmm Orthorhombic

No. 64 $C\ 2/m\ 2/c\ 2_1/e$ Patterson symmetry $Cmmm$

Former space-group symbol $Cmca$; *cf.* Section 2.1.2



Origin at centre $(2/m)$ at $2/mn1$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) b $x,y,\frac{1}{4}$	(7) c $x,\frac{1}{4},z$	(8) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) a $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			General:
16	*g*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*f*	*m* . .	$0,y,z$	$0,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*e*	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{4}$	hkl: $h=2n$
8	*d*	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$	$x,\frac{1}{2},\frac{1}{2}$	hkl: $k+l=2n$
8	*c*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	hkl: $k,l=2n$
4	*b*	2/*m* . .	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$
4	*a*	2/*m* . .	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

Symmetry of special projections

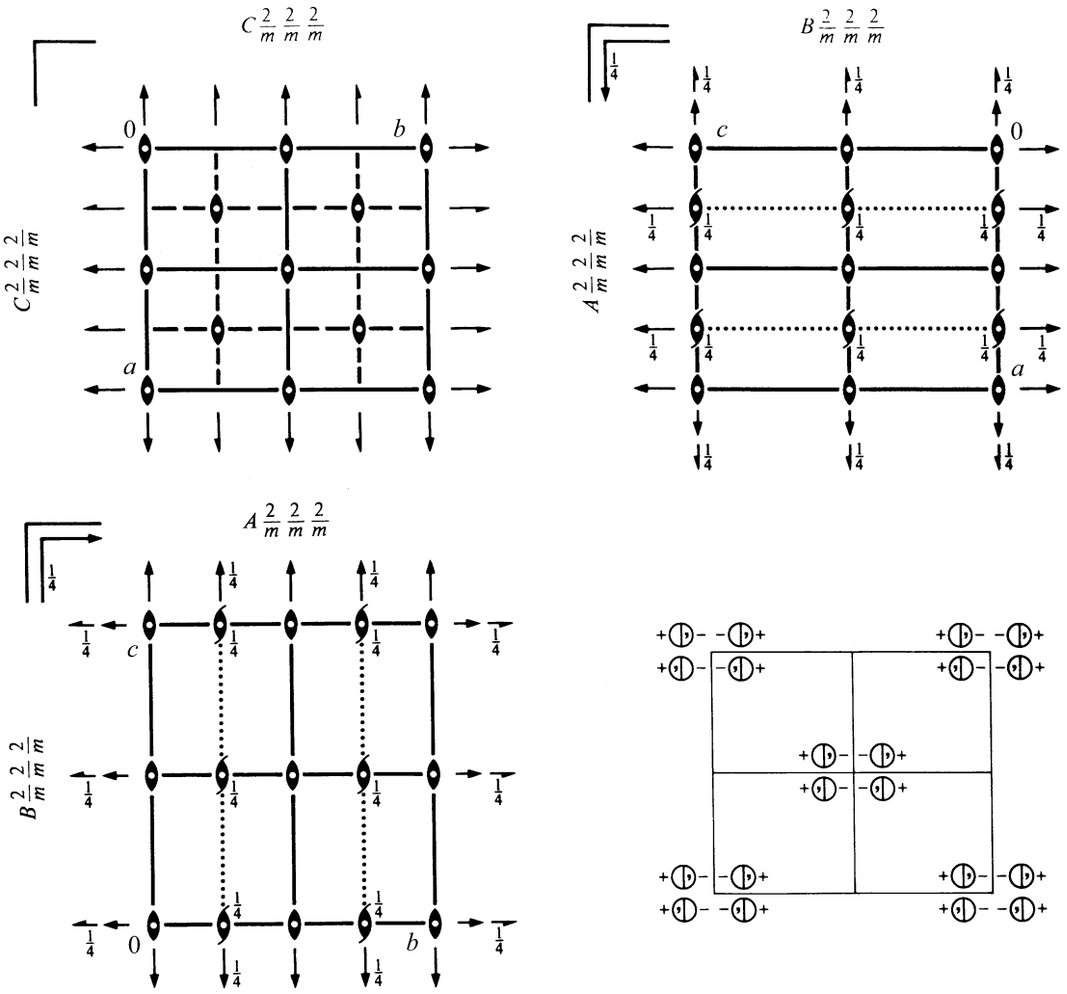
Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Cmmm$ D_{2h}^{19} mmm Orthorhombic

No. 65 $C\ 2/m\ 2/m\ 2/m$ Patterson symmetry $Cmmm$



Origin at centre (mmm)

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) m $x,0,z$	(8) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) a $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	*r*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
8	*q*	. . *m*	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	*p*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
8	*o*	. *m* .	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
8	*n*	*m* . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*m*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z$	hkl: $h=2n$
4	*l*	*m m* 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			no extra conditions
4	*k*	*m m* 2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	*j*	*m* 2 *m*	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	*i*	*m* 2 *m*	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	*h*	2 *m m*	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			no extra conditions
4	*g*	2 *m m*	$x,0,0$	$\bar{x},0,0$			no extra conditions
4	*f*	. . 2/*m*	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $h=2n$
4	*e*	. . 2/*m*	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl: $h=2n$
2	*d*	*m m m*	$0,0,\frac{1}{2}$				no extra conditions
2	*c*	*m m m*	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	*b*	*m m m*	$\frac{1}{2},0,0$				no extra conditions
2	*a*	*m m m*	$0,0,0$				no extra conditions

Symmetry of special projections

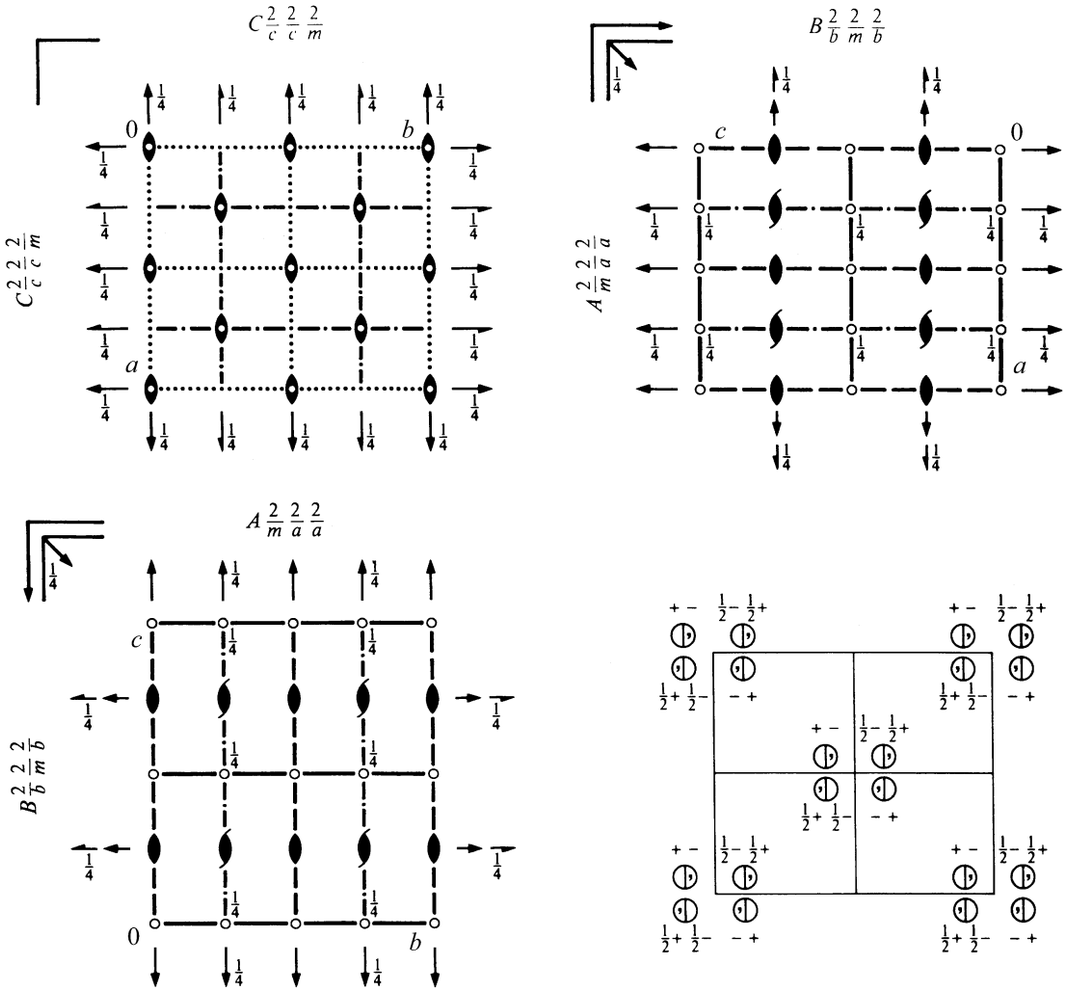
Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Cccm$ D_{2h}^{20} mmm Orthorhombic

No. 66 $C\ 2/c\ 2/c\ 2/m$ Patterson symmetry $Cmmm$



Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) 2 $x,0,\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) c $x,0,z$	(8) c $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},0)+$			Reflection conditions
							General:
16	*m*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$	hkl: $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*l*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	*k*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	*j*	. . 2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	*i*	. . 2	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	*h*	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	*g*	2 . .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
4	*f*	. . 2/*m*	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	*e*	. . 2/*m*	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	*d*	. . 2/*m*	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	*c*	. . 2/*m*	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
4	*b*	2 2 2	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	*a*	2 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

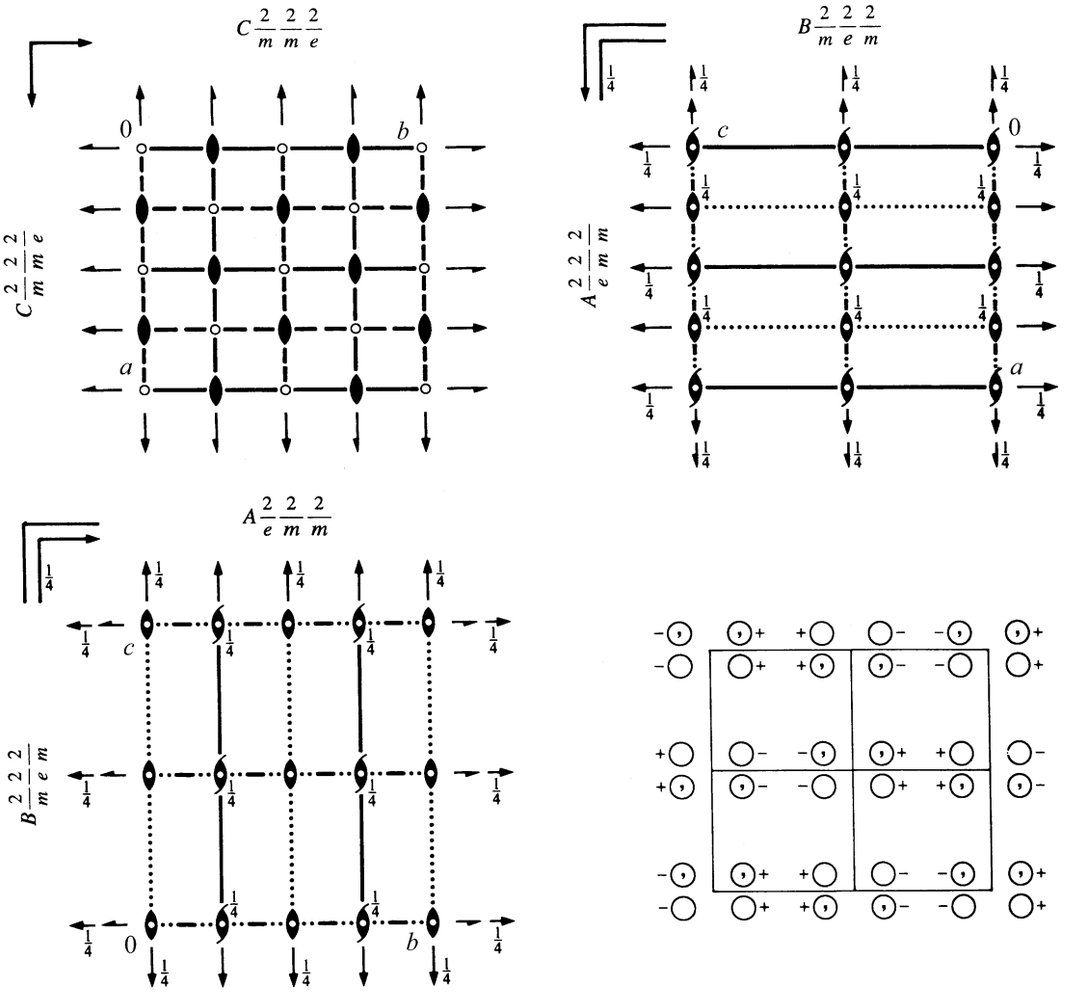
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Cmme$ D_{2h}^{21} *mmm* Orthorhombic

No. 67 $C\ 2/m\ 2/m\ 2/e$ Patterson symmetry $Cmmm$

Former space-group symbol $Cmma$; *cf.* Section 2.1.2



Origin at centre $(2/m)$ at $2/m2_1/ae$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) b $x,y,0$	(7) m $x,\frac{1}{4},z$	(8) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) a $x,y,0$	(7) a $x,0,z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	*o*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z$ (6) $x,y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
8	*n*	. *m* .	$x,\frac{1}{4},z$	$\bar{x},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x,\frac{3}{4},\bar{z}$	no extra conditions
8	*m*	*m* . .	$0,y,z$	$0,\bar{y}+\frac{1}{2},z$	$0,y+\frac{1}{2},\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*l*	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},\frac{1}{2},\bar{z}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},\frac{1}{2},z$	hkl: $h=2n$
8	*k*	. 2 .	$\frac{1}{4},y,\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{3}{4},\bar{y},\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},\frac{1}{2}$	hkl: $h=2n$
8	*j*	. 2 .	$\frac{1}{4},y,0$	$\frac{3}{4},\bar{y}+\frac{1}{2},0$	$\frac{3}{4},\bar{y},0$	$\frac{1}{4},y+\frac{1}{2},0$	hkl: $h=2n$
8	*i*	2 . .	$x,0,\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$x,\frac{1}{2},\frac{1}{2}$	hkl: $h=2n$
8	*h*	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},0$	$\bar{x},0,0$	$x,\frac{1}{2},0$	hkl: $h=2n$
4	*g*	*m m* 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4	*f*	. 2/*m* .	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $h=2n$
4	*e*	. 2/*m* .	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl: $h=2n$
4	*d*	2/*m* . .	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h=2n$
4	*c*	2/*m* . .	$0,0,0$	$0,\frac{1}{2},0$			hkl: $h=2n$
4	*b*	2 2 2	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$			hkl: $h=2n$
4	*a*	2 2 2	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$			hkl: $h=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

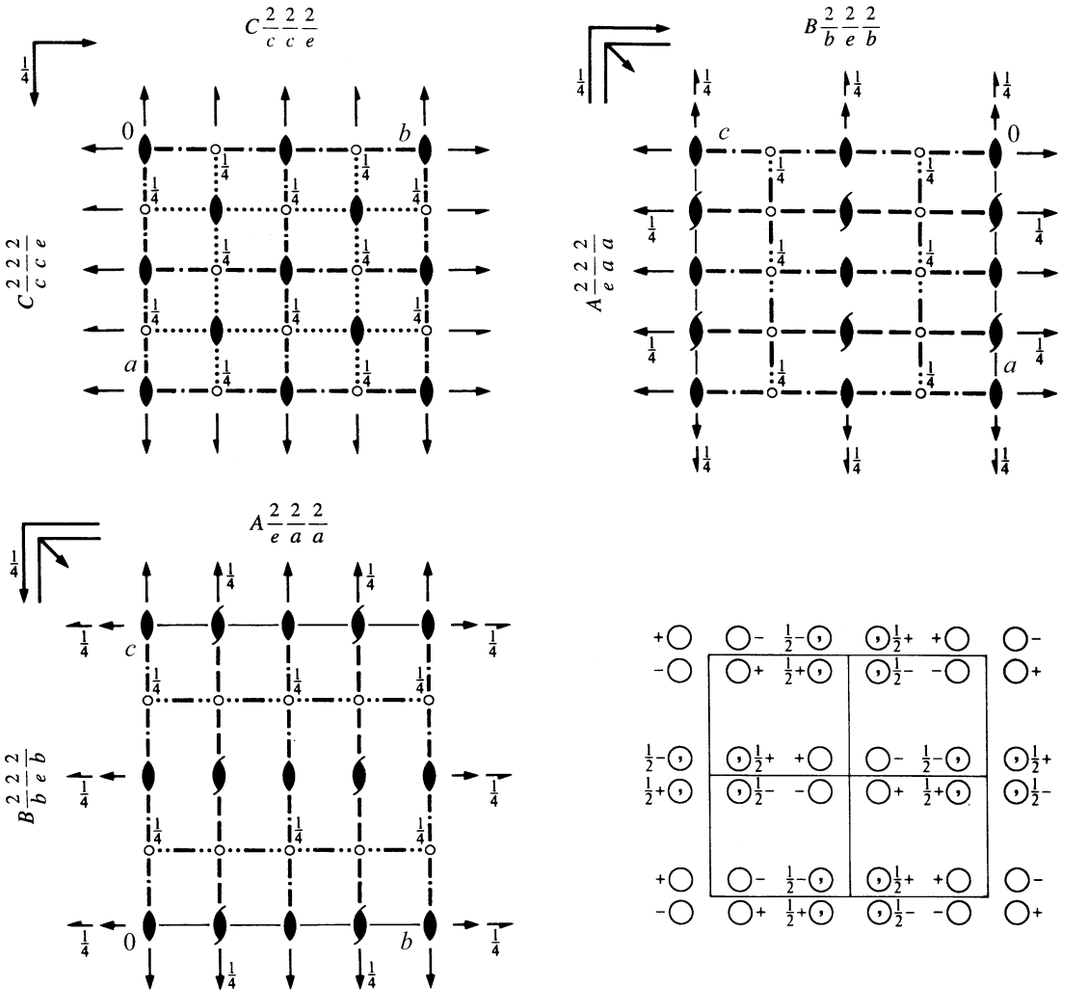
International Tables for Crystallography (2016). Vol. A, Space group 68, pp. 366–369.

$Ccce$ D_{2h}^{22} *mmm* Orthorhombic

No. 68 $C\ 2/c\ 2/c\ 2/e$ Patterson symmetry $Cmmm$

Former space-group symbol $Ccca$; *cf.* Section 2.1.2

ORIGIN CHOICE 1



Origin at 222 at $2/n2/n2$, at $0,\frac{1}{4},\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $0,y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$	(6) a $x,y,\frac{1}{4}$	(7) c $x,\frac{1}{4},z$	(8) c $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $0,0,z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$	(6) b $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+	(½,½,0)+			Reflection conditions
							General:
16	*i*	1	(1) x,y,z (5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	hkl: $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*h*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	hkl: $l=2n$
8	*g*	. . 2	$0,0,z$	$0,0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $k+l=2n$
8	*f*	. 2 .	$0,y,0$	$\frac{1}{2},\bar{y}+\frac{1}{2},0$	$0,\bar{y}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},y,\frac{1}{2}$	hkl: $k+l=2n$
8	*e*	2 . .	$x,0,0$	$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},0,\frac{1}{2}$	hkl: $k+l=2n$
8	*d*	$\bar{1}$	$0,\frac{1}{4},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	hkl: $k,l=2n$
8	*c*	$\bar{1}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{3}{4}$	$\frac{3}{4},\frac{1}{2},\frac{3}{4}$	hkl: $k,l=2n$
4	*b*	2 2 2	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl: $k+l=2n$
4	*a*	2 2 2	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $k+l=2n$

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

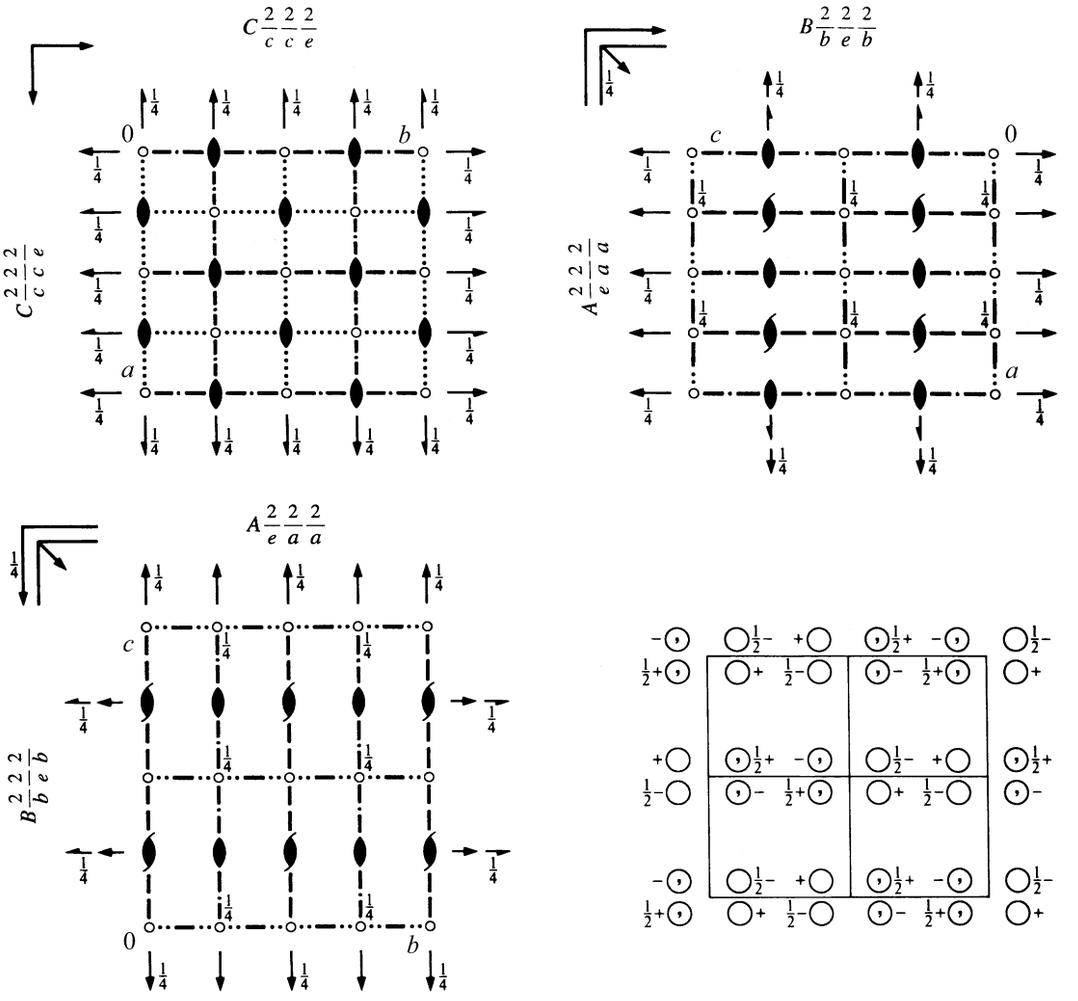
Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

No. 68 $C\ 2/c\ 2/c\ 2/e$

Patterson symmetry $Cmmm$

Former space-group symbol $Ccca$; *cf.* Section 2.1.2

ORIGIN CHOICE 2



Origin at $\bar{1}$ at nce, at $0, -\frac{1}{4}, -\frac{1}{4}$ from 222

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $\frac{1}{4},0,z$	(3) 2 $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,0$	(7) c $x,0,z$	(8) c $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) b $x,y,0$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	*i*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z$ (6) $x+\frac{1}{2},y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	hkl: $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*h*	. . 2	$\frac{1}{4},0,z$	$\frac{3}{4},0,\bar{z}+\frac{1}{2}$	$\frac{3}{4},0,\bar{z}$	$\frac{1}{4},0,z+\frac{1}{2}$	hkl: $l=2n$
8	*g*	. . 2	$0,\frac{1}{4},z$	$0,\frac{1}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	*f*	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y,\frac{3}{4}$	hkl: $k+l=2n$
8	*e*	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	hkl: $k+l=2n$
8	*d*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $k,l=2n$
8	*c*	$\bar{1}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl: $k,l=2n$
4	*b*	2 2 2	$0,\frac{1}{4},\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl: $k+l=2n$
4	*a*	2 2 2	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{3}{4}$			hkl: $k+l=2n$

Symmetry of special projections

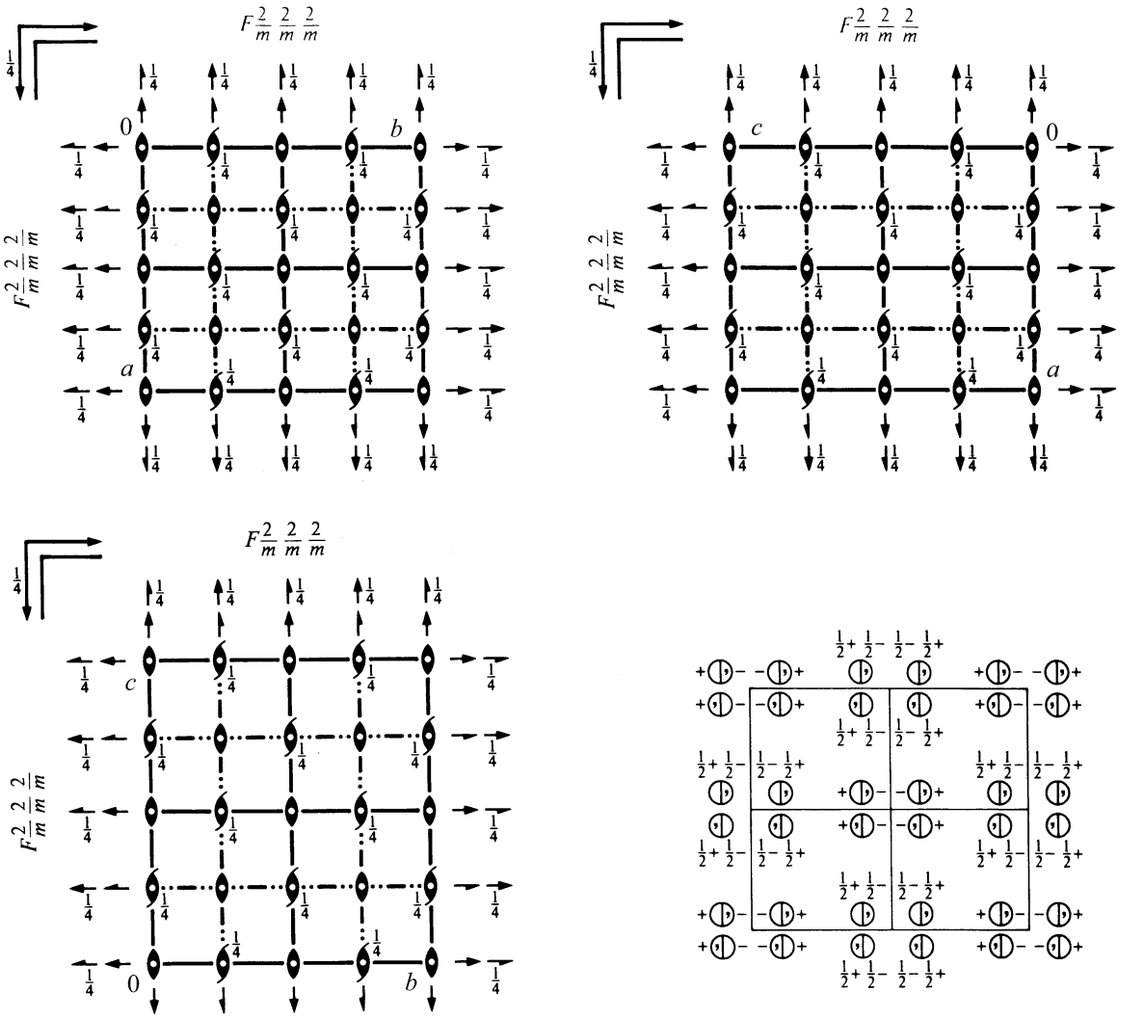
Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$F\,m\,m\,m$ D_{2h}^{23} $m\,m\,m$ Orthorhombic

No. 69 $F\ 2/m\ 2/m\ 2/m$ Patterson symmetry $F\,m\,m\,m$



Origin at centre $(m\,m\,m)$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) m $x,0,z$	(8) m $0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$	(6) b $x,y,\frac{1}{4}$	(7) c $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$	(6) a $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(8) c $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) a $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							General:
32	p	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
16	o	. . m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
16	n	. m .	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
16	m	m . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
16	l	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	hkl: $h=2n$
16	k	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y,\frac{3}{4}$	hkl: $h=2n$
16	j	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z$	hkl: $h=2n$
8	i	m m 2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
8	h	m 2 m	$0,y,0$	$0,\bar{y},0$			no extra conditions
8	g	2 m m	$x,0,0$	$\bar{x},0,0$			no extra conditions
8	f	2 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h=2n$
8	e	. . 2/m	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl: $h=2n$
8	d	. 2/m .	$\frac{1}{4},0,\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$			hkl: $h=2n$
8	c	2/m . .	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$			hkl: $h=2n$
4	b	m m m	$0,0,\frac{1}{2}$				no extra conditions
4	a	m m m	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

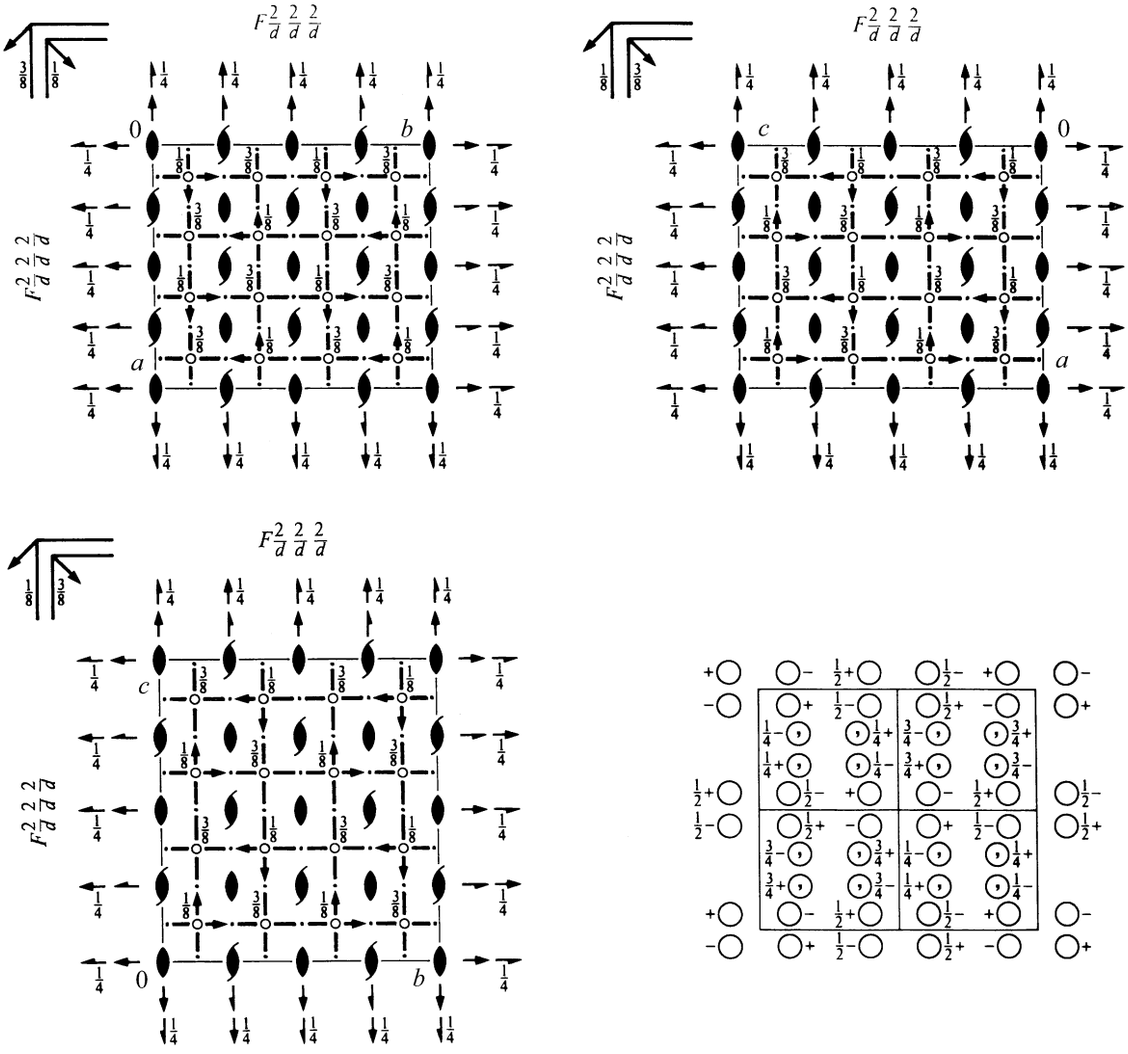
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$F\,d\,d\,d$ D_{2h}^{24} *mmm* Orthorhombic

No. 70 $F\ 2/d\ 2/d\ 2/d$ Patterson symmetry $F\,m\,m\,m$

ORIGIN CHOICE 1



Origin at 222, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{8}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$	(6) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,\frac{1}{8}$	(7) $d(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},z$	(8) $d(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{8},\frac{3}{8},\frac{3}{8}$	(6) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{3}{8}$	(7) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{3}{8},z$	(8) $d(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $\bar{1}$ $\frac{3}{8},\frac{1}{8},\frac{3}{8}$	(6) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{3}{8}$	(7) $d(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},z$	(8) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{3}{8},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $\frac{3}{8},\frac{3}{8},\frac{1}{8}$	(6) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,\frac{1}{8}$	(7) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{3}{8},z$	(8) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{3}{8},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
32	*h*	1	(1) x,y,z (5) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(3) $\bar{x},y,\bar{z}$ (7) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$	General: *hkl*: $h+k=2n$ and $h+l,k+l=2n$ 0*kl*: $k+l=4n$ and $k,l=2n$ *h*0*l*: $h+l=4n$ and $h,l=2n$ *hk*0: $h+k=4n$ and $h,k=2n$ *h*00: $h=4n$ 0*k*0: $k=4n$ 00*l*: $l=4n$
							Special: as above, plus
16	*g*	. . 2	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{4}$	*hkl*: $h=2n+1$ or $h+k+l=4n$
16	*f*	. 2 .	$0,y,0$	$0,\bar{y},0$	$\frac{1}{4},\bar{y}+\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},y+\frac{1}{4},\frac{1}{4}$	
16	*e*	2 . .	$x,0,0$	$\bar{x},0,0$	$\bar{x}+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$x+\frac{1}{4},\frac{1}{4},\frac{1}{4}$	
16	*d*	$\bar{1}$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{3}{8}$	*hkl*: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	*c*	$\bar{1}$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{7}{8}$	
8	*b*	2 2 2	$0,0,\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$			*hkl*: $h=2n+1$ or $h+k+l=4n$
8	*a*	2 2 2	$0,0,0$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$			

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

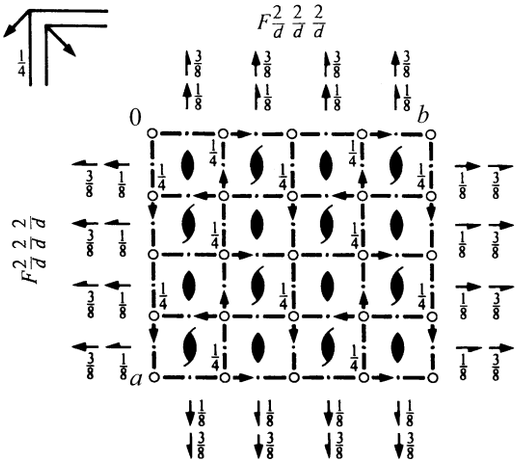
Along [100] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

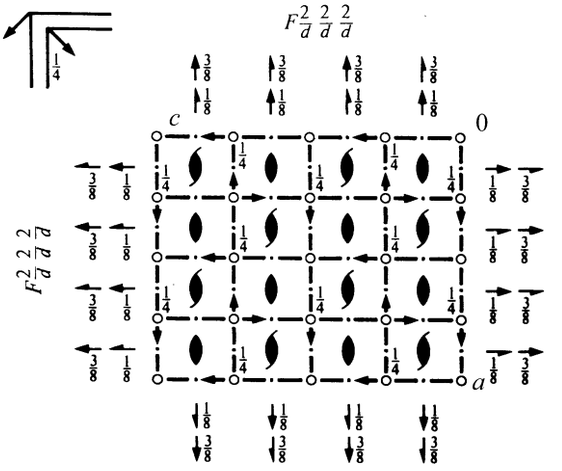
Along [010] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

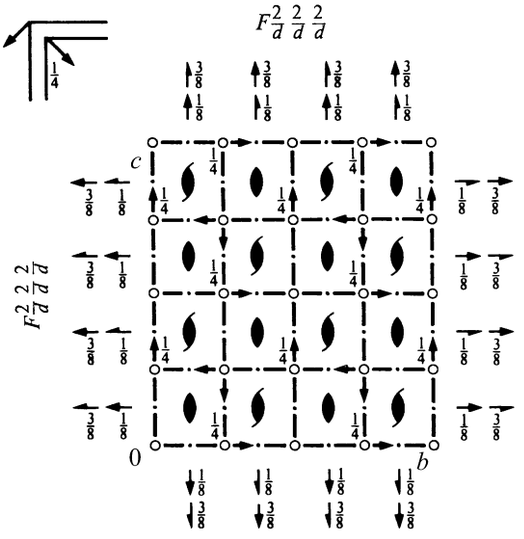
No. 70 $F\ 2/d\ 2/d\ 2/d$

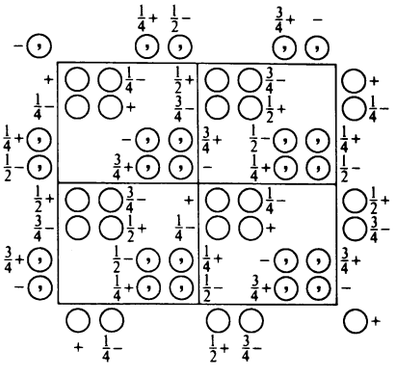
Patterson symmetry $F\,m\,m\,m$

ORIGIN CHOICE 2









Origin at $\bar{1}$ at $d\,d\,d$, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from $2\,2\,2$

Asymmetric unit $0 \le x \le \frac{1}{8}; \quad -\frac{1}{8} \le y \le \frac{1}{8}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\ \frac{3}{8},\frac{3}{8},z$	(3) $2\ \frac{3}{8},y,\frac{3}{8}$	(4) $2\ x,\frac{3}{8},\frac{3}{8}$
(5) $\bar{1}\ \ 0,0,0$	(6) $d(\frac{1}{4},\frac{1}{4},0)\ \ x,y,0$	(7) $d(\frac{1}{4},0,\frac{1}{4})\ \ x,0,z$	(8) $d(0,\frac{1}{4},\frac{1}{4})\ \ 0,y,z$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \frac{3}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\ \frac{3}{8},y,\frac{1}{8}$	(4) $2\ x,\frac{1}{8},\frac{1}{8}$
(5) $\bar{1}\ \ 0,\frac{1}{4},\frac{1}{4}$	(6) $d(\frac{1}{4},\frac{3}{4},0)\ \ x,y,\frac{1}{4}$	(7) $d(\frac{1}{4},0,\frac{3}{4})\ \ x,\frac{1}{4},z$	(8) $d(0,\frac{3}{4},\frac{3}{4})\ \ 0,y,z$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \frac{1}{8},\frac{3}{8},z$	(3) $2\ \frac{1}{8},y,\frac{1}{8}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{3}{8},\frac{1}{8}$
(5) $\bar{1}\ \ \frac{1}{4},0,\frac{1}{4}$	(6) $d(\frac{3}{4},\frac{1}{4},0)\ \ x,y,\frac{1}{4}$	(7) $d(\frac{3}{4},0,\frac{3}{4})\ \ x,0,z$	(8) $d(0,\frac{1}{4},\frac{3}{4})\ \ \frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\ \frac{1}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)\ \frac{1}{8},y,\frac{3}{8}$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{8},\frac{3}{8}$
(5) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},0$	(6) $d(\frac{3}{4},\frac{3}{4},0)\ \ x,y,0$	(7) $d(\frac{3}{4},0,\frac{1}{4})\ \ x,\frac{1}{4},z$	(8) $d(0,\frac{3}{4},\frac{1}{4})\ \ \frac{1}{4},y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							General:
32	*h*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},z$ (6) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}$	(3) $\bar{x}+\frac{3}{4},y,\bar{z}+\frac{3}{4}$ (7) $x+\frac{1}{4},\bar{y},z+\frac{1}{4}$	(4) $x,\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$ (8) $\bar{x},y+\frac{1}{4},z+\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$ $0kl$: $k+l=4n$, $k,l=2n$ $h0l$: $h+l=4n$, $h,l=2n$ $hk0$: $h+k=4n$, $h,k=2n$ $h00$: $h=4n$ $0k0$: $k=4n$ $00l$: $l=4n$
							Special: as above, plus
16	*g*	. . 2	$\frac{1}{8},\frac{1}{8},z$	$\frac{5}{8},\frac{1}{8},\bar{z}+\frac{3}{4}$	$\frac{7}{8},\frac{7}{8},\bar{z}$	$\frac{3}{8},\frac{7}{8},z+\frac{1}{4}$	hkl: $h=2n+1$ or $h+k+l=4n$
16	*f*	. 2 .	$\frac{1}{8},y,\frac{1}{8}$	$\frac{5}{8},\bar{y}+\frac{3}{4},\frac{1}{8}$	$\frac{7}{8},\bar{y},\frac{7}{8}$	$\frac{3}{8},y+\frac{1}{4},\frac{7}{8}$	
16	*e*	2 . .	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{5}{8},\frac{1}{8}$	$\bar{x},\frac{7}{8},\frac{7}{8}$	$x+\frac{1}{4},\frac{3}{8},\frac{7}{8}$	
16	*d*	$\bar{1}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$	hkl: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	*c*	$\bar{1}$	$0,0,0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{3}{4}$	$0,\frac{3}{4},\frac{3}{4}$	
8	*b*	2 2 2	$\frac{1}{8},\frac{1}{8},\frac{5}{8}$	$\frac{7}{8},\frac{7}{8},\frac{3}{8}$			hkl: $h=2n+1$ or $h+k+l=4n$
8	*a*	2 2 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$			

Symmetry of special projections

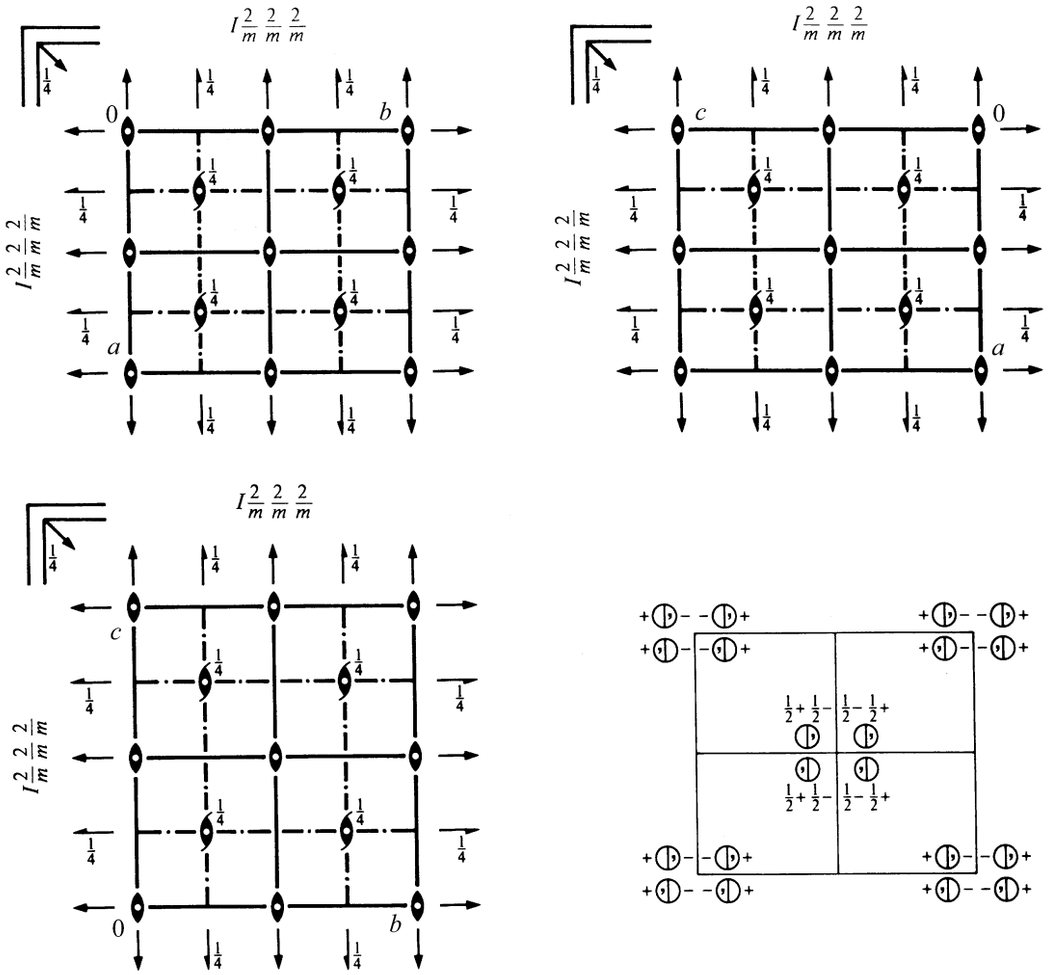
Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{8},\frac{1}{8},z$

Along [100] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{8},\frac{1}{8}$

Along [010] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \frac{1}{2}\mathbf{a}$
Origin at $\frac{1}{8},y,\frac{1}{8}$

$Immm$ D_{2h}^{25} mmm Orthorhombic

No. 71 $I\ 2/m\ 2/m\ 2/m$ Patterson symmetry $Immm$



Origin at centre (mmm)

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) m $x,0,z$	(8) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:
16	*o*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}$ (7) $x,\bar{y},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*n*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions
8	*m*	. *m* .	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	no extra conditions
8	*l*	*m* . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*k*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	hkl: $k,l=2n$
4	*j*	*m m* 2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
4	*i*	*m m* 2	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	*h*	*m* 2 *m*	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			no extra conditions
4	*g*	*m* 2 *m*	$0,y,0$	$0,\bar{y},0$			no extra conditions
4	*f*	2 *m m*	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			no extra conditions
4	*e*	2 *m m*	$x,0,0$	$\bar{x},0,0$			no extra conditions
2	*d*	*m m m*	$\frac{1}{2},0,\frac{1}{2}$				no extra conditions
2	*c*	*m m m*	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	*b*	*m m m*	$0,\frac{1}{2},\frac{1}{2}$				no extra conditions
2	*a*	*m m m*	$0,0,0$				no extra conditions

Symmetry of special projections

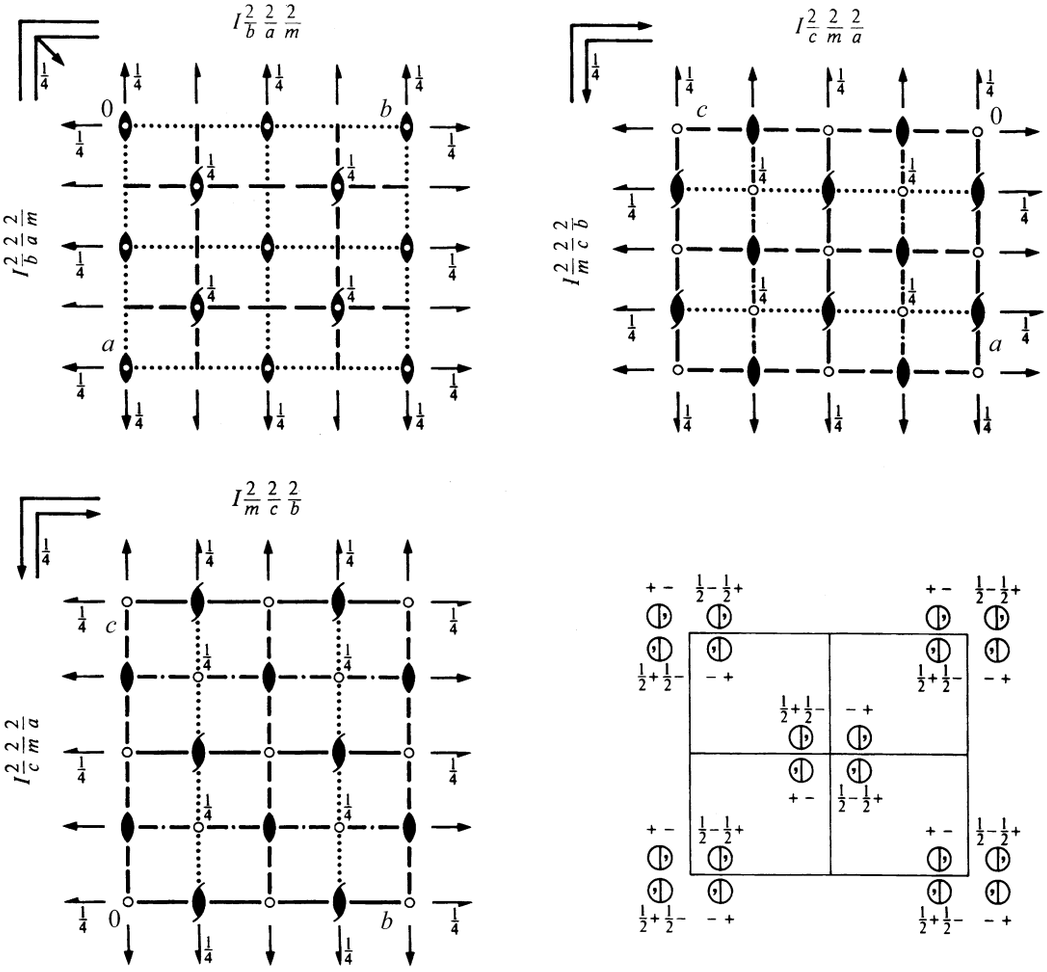
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $c2mm$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

$Ibam$ D_{2h}^{26} mmm Orthorhombic

No. 72 $I\ 2/b\ 2/a\ 2/m$ Patterson symmetry $Immm$



Origin at centre $(2/m)$ at $cc2/m$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) a $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) 2 $0,y,\frac{1}{4}$	(4) 2 $x,0,\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) c $x,0,z$	(8) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
16	k	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (7) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	General: hkl: $h+k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	j	. . m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	no extra conditions
8	i	. . 2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl: $l=2n$
8	h	. . 2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl: $l=2n$
8	g	. 2 .	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	f	2 . .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl: $k,l=2n$
4	d	. . 2/m	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl: $l=2n$
4	c	. . 2/m	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $l=2n$
4	b	2 2 2	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl: $l=2n$
4	a	2 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

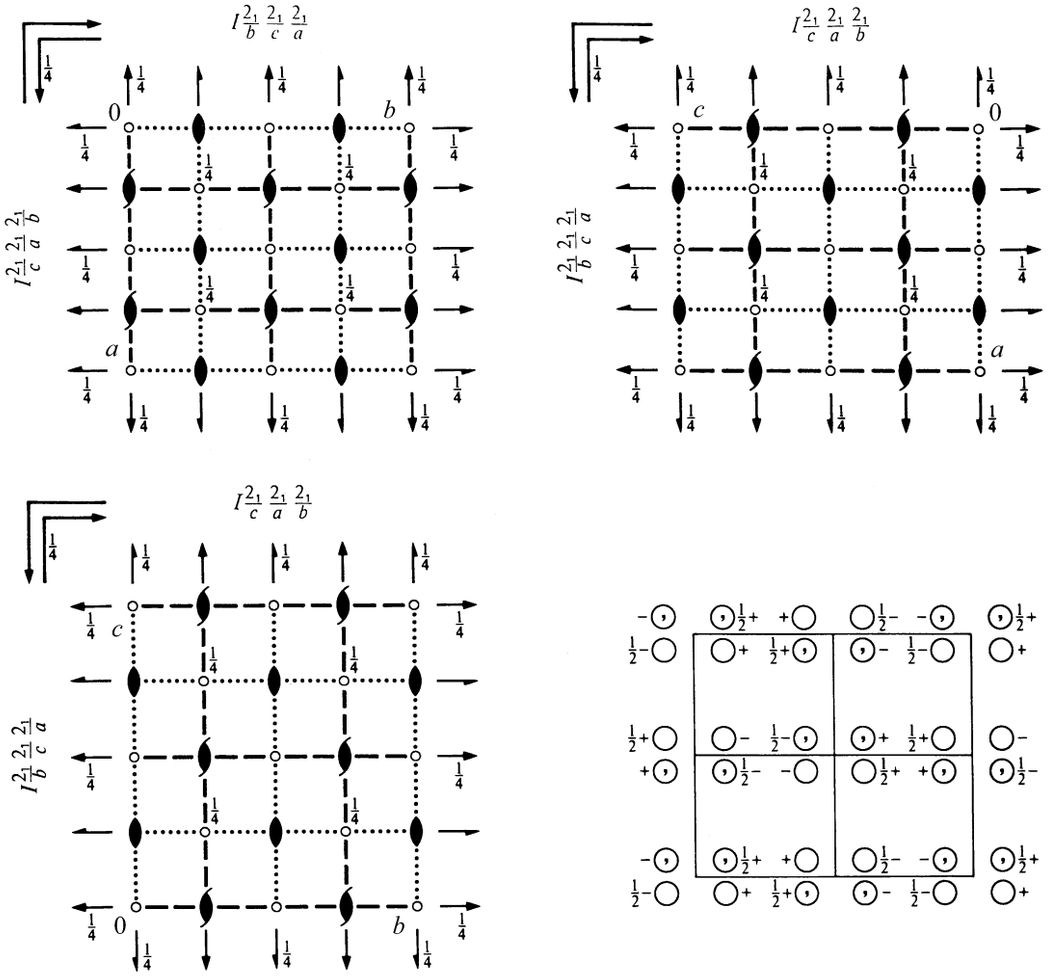
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Ibca$ D_{2h}^{27} mmm Orthorhombic

No. 73 $I\ 2_1/b\ 2_1/c\ 2_1/a$ Patterson symmetry $Immm$



Origin at $\bar{1}$ at cab

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) c $x,\frac{1}{4},z$	(8) b $\frac{1}{4},y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,0$	(4) 2 $x,0,\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) b $x,y,0$	(7) a $x,0,z$	(8) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	*f*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hkl: $h+k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*e*	. . 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{1}{4},z+\frac{1}{2}$	hkl: $l=2n$
8	*d*	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y,\frac{1}{2}$	hkl: $k=2n$
8	*c*	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	hkl: $h=2n$
8	*b*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl: $k,l=2n$
8	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $k,l=2n$

Symmetry of special projections

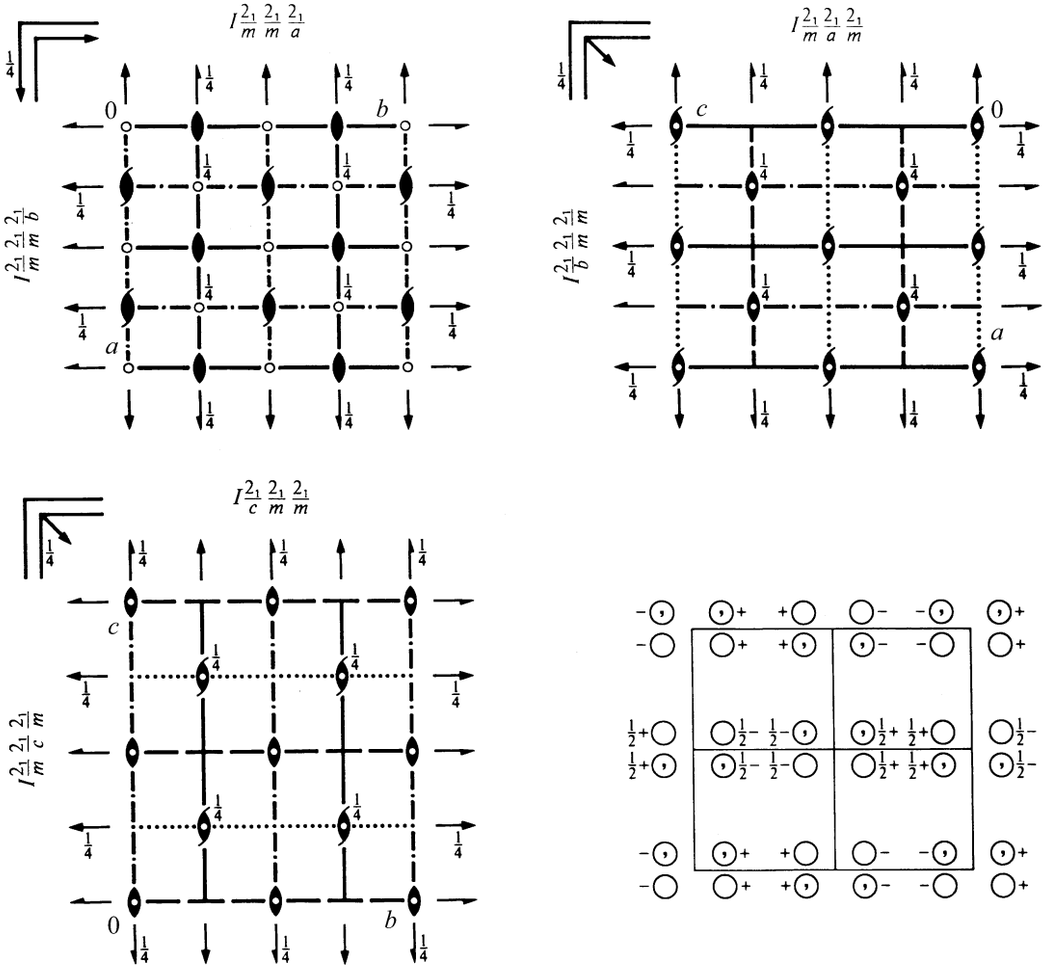
Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

$Imma$ D_{2h}^{28} mmm Orthorhombic

No. 74 $I\ 2_1/m\ 2_1/m\ 2_1/a$ Patterson symmetry $Immm$



Origin at centre $(2/m)$ at $2/m2_1/nb$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $0,y,0$	(4) 2 $x,0,0$
(5) $\bar{1}$ $0,0,0$	(6) b $x,y,0$	(7) m $x,\frac{1}{4},z$	(8) m $0,y,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) a $x,y,\frac{1}{4}$	(7) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	*j*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y}+\frac{1}{2},z$ (6) $x,y+\frac{1}{2},\bar{z}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{x},y,z$	hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ $h0l$: $h+l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*i*	. *m* .	$x,\frac{1}{4},z$	$\bar{x},\frac{1}{4},z$	$\bar{x},\frac{3}{4},\bar{z}$	$x,\frac{3}{4},\bar{z}$	no extra conditions
8	*h*	*m* . .	$0,y,z$	$0,\bar{y}+\frac{1}{2},z$	$0,y+\frac{1}{2},\bar{z}$	$0,\bar{y},\bar{z}$	no extra conditions
8	*g*	. 2 .	$\frac{1}{4},y,\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{y},\frac{3}{4}$	$\frac{1}{4},y+\frac{1}{2},\frac{3}{4}$	hkl: $h=2n$
8	*f*	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},0$	$\bar{x},0,0$	$x,\frac{1}{2},0$	hkl: $k=2n$
4	*e*	*m m* 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}$			no extra conditions
4	*d*	. 2/*m* .	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			hkl: $h=2n$
4	*c*	. 2/*m* .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl: $h=2n$
4	*b*	2/*m* . .	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h=2n$
4	*a*	2/*m* . .	$0,0,0$	$0,\frac{1}{2},0$			hkl: $h=2n$

Symmetry of special projections

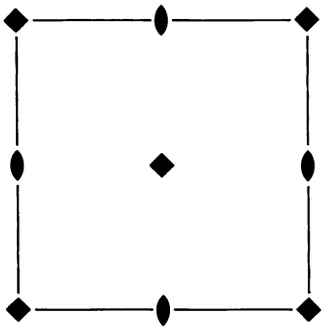
Along [001] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

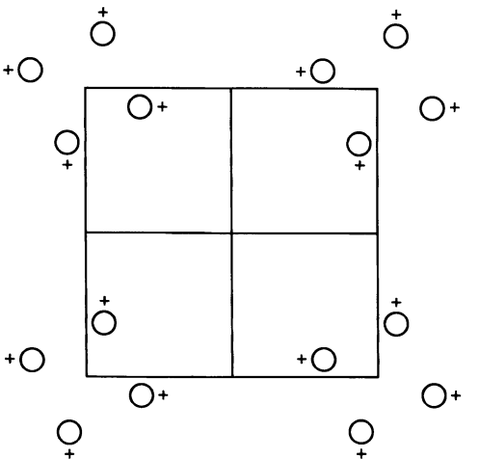
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $c2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

$P4$ C_4^1 4 Tetragonal

No. 75 $P4$ Patterson symmetry $P4/m$





Origin on 4

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	no conditions
							Special:
2	c	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl: $h+k=2n$
1	b	4 . .	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	4 . .	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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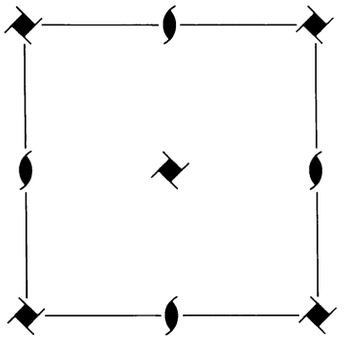
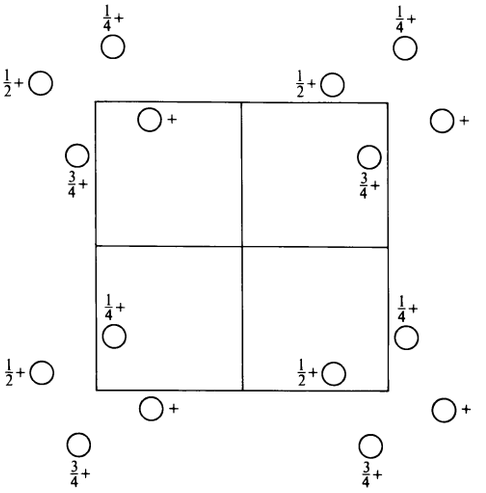
Tetragonal 4 C_4^2 $P4_1$

Patterson symmetry $P4/m$ $P4_1$ No. 76





Origin on 4_1

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{1}{4})$ $0,0,z$ (4) $4^-(0,0,\frac{3}{4})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
4	*a*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$	$00l$: $l = 4n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1g1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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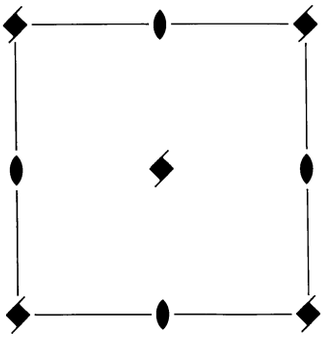
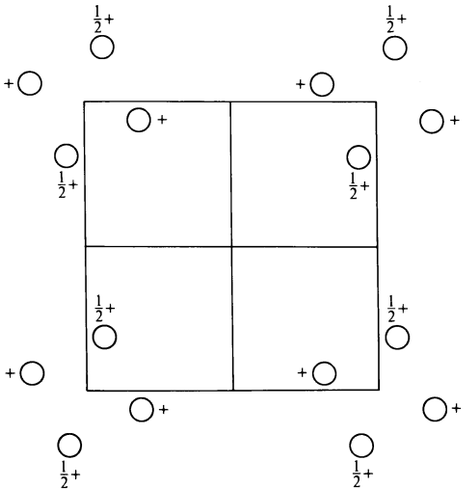
$P4_2$ C_4^3 4 Tetragonal

No. 77 $P4_2$ Patterson symmetry $P4/m$





Origin on 2 on 4_2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 d 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$00l$: $l=2n$
					Special: as above, plus
2 c 2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl: $h+k+l=2n$
2 b 2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $l=2n$
2 a 2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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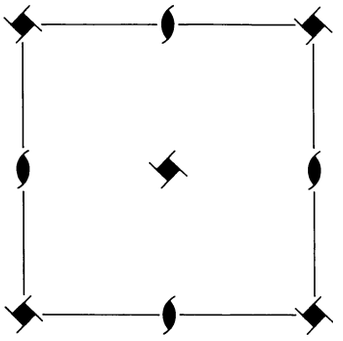
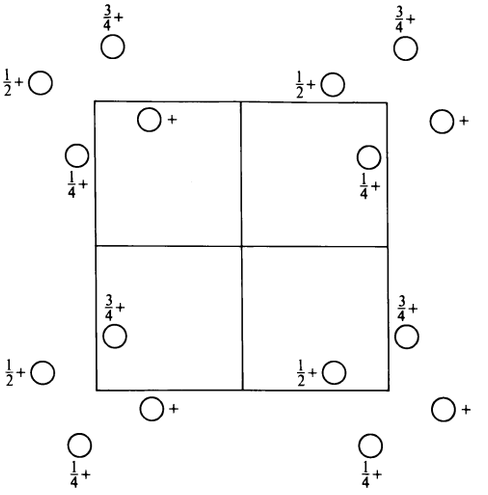
Tetragonal 4 C_4^4 $P4_3$

Patterson symmetry $P4/m$ $P4_3$ No. 78





Origin on 4_3

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{3}{4})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{4})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 a 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{3}{4}$	(4) $y,\bar{x},z+\frac{1}{4}$	$00l$: $l = 4n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1g1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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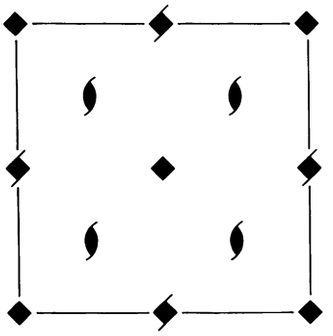
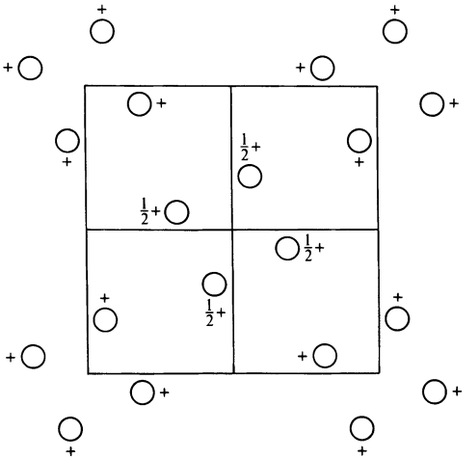
$I\,4$ C_4^5 4 Tetragonal

No. 79 $I\,4$ Patterson symmetry $I\,4/m$





Origin on 4

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
						General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$ (4) $y,\bar{x},z$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
						Special: as above, plus
4	b	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$		hkl: $l=2n$
2	a	4 . .	$0,0,z$			no extra conditions

Symmetry of special projections

Along [001] $p\,4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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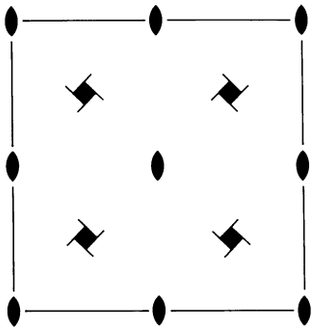
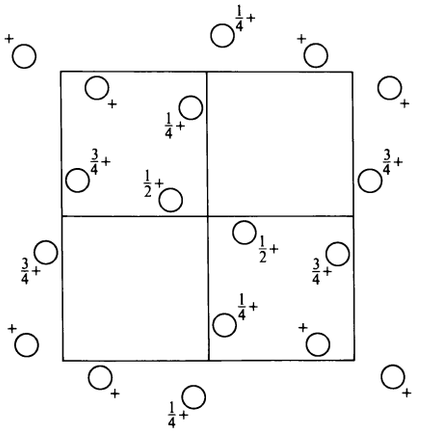
Tetragonal 4 C_4^6 $I4_1$

Patterson symmetry $I4/m$ $I4_1$ No. 80





Origin on 2

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$ (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$ (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
					General:
8 *b* 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	*hkl*: $h+k+l=2n$ *hk*0: $h+k=2n$ 0*kl*: $k+l=2n$ *hhl*: $l=2n$ 00*l*: $l=4n$ *h*00: $h=2n$
					Special: as above, plus
4 *a* 2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$			*hkl*: $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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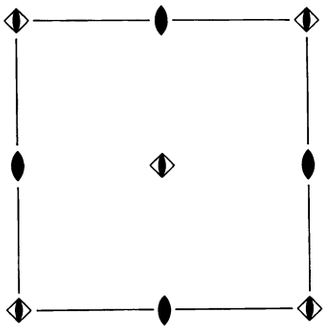
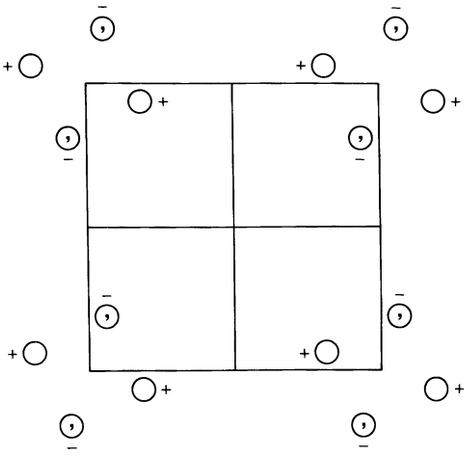
$P\bar{4}$ S_4^1 $\bar{4}$ Tetragonal

No. 81 $P\bar{4}$ Patterson symmetry $P4/m$





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ (4) $\bar{4}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	no conditions
							Special:
2	g	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	f	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	e	2 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
1	d	$\bar{4}$ . .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	$\bar{4}$ . .	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$				no extra conditions
1	a	$\bar{4}$ . .	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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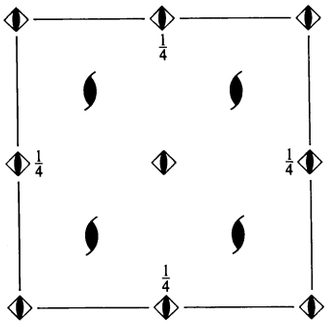
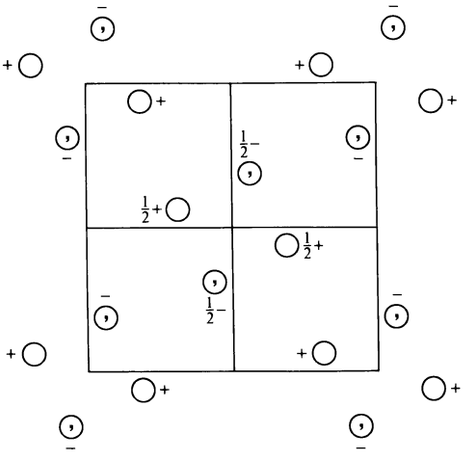
Tetragonal $\bar{4}$ S_4^2 $I\bar{4}$

Patterson symmetry $I4/m$ $I\bar{4}$ No. 82





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ (4) $\bar{4}^-$ $0,0,z$; $0,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$ (4) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	General:
							hkl: $h+k+l=2n$
							$hk0$: $h+k=2n$
							$0kl$: $k+l=2n$
							hhl: $l=2n$
							$00l$: $l=2n$
							$h00$: $h=2n$
							Special: no extra conditions
4	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			
4	e	2 . .	$0,0,z$	$0,0,\bar{z}$			
2	d	$\bar{4}$ . .	$0,\frac{1}{2},\frac{3}{4}$				
2	c	$\bar{4}$ . .	$0,\frac{1}{2},\frac{1}{4}$				
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$				
2	a	$\bar{4}$ . .	$0,0,0$				

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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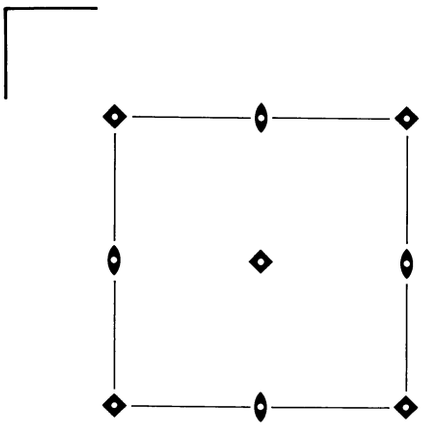
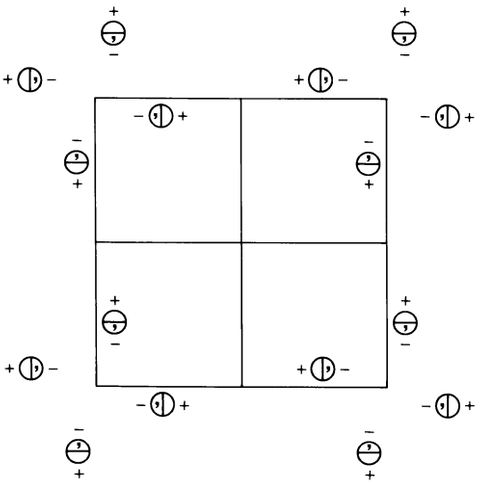
$P4/m$ C_{4h}^{1} $4/m$ Tetragonal

No. 83 $P4/m$ Patterson symmetry $P4/m$





Origin at centre $(4/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$
(5) $\bar{1}$ $0,0,0$ (6) m $x,y,0$ (7) $\bar{4}^+$ $0,0,z$; $0,0,0$ (8) $\bar{4}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	l	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$	no conditions
							Special:
4	k	m . .	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
4	j	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
4	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $h+k=2n$
2	h	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	$2/m$ . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
2	e	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
1	d	$4/m$ . .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	$4/m$ . .	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	$4/m$ . .	$0,0,\frac{1}{2}$				no extra conditions
1	a	$4/m$ . .	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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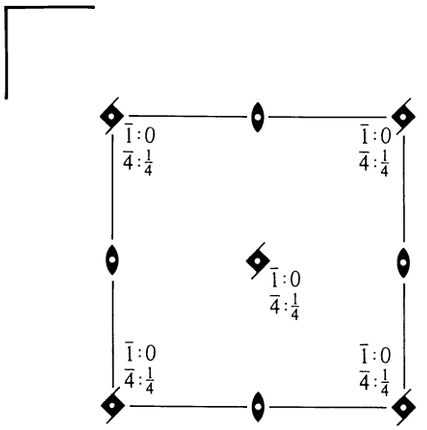
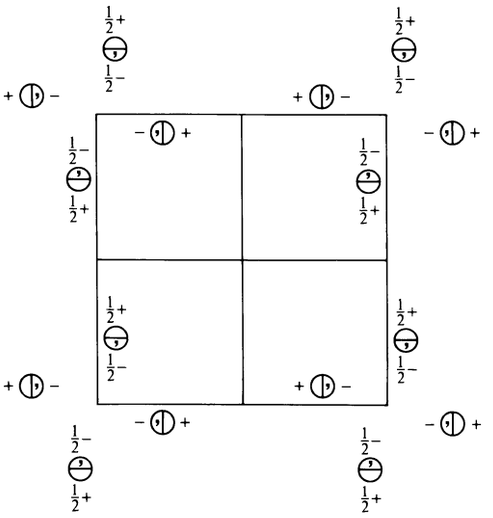
Tetragonal $4/m$ C_{4h}^2 $P4_2/m$

Patterson symmetry $P4/m$ $P4_2/m$ No. 84





Origin at centre $(2/m)$ on 4_2

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) $\bar{1}$ $0,0,0$ (6) m $x,y,0$ (7) $\bar{4}^+$ $0,0,z$; $0,0,\frac{1}{4}$ (8) $\bar{4}^-$ $0,0,z$; $0,0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	k	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $y,\bar{x},\bar{z}+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $\bar{y},x,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
4	j	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
4	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
4	h	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	g	2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
2	f	$\bar{4}$ . .	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	e	$\bar{4}$ . .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$
2	d	$2/m$ . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl: $h+k+l=2n$
2	c	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	b	$2/m$ . .	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	a	$2/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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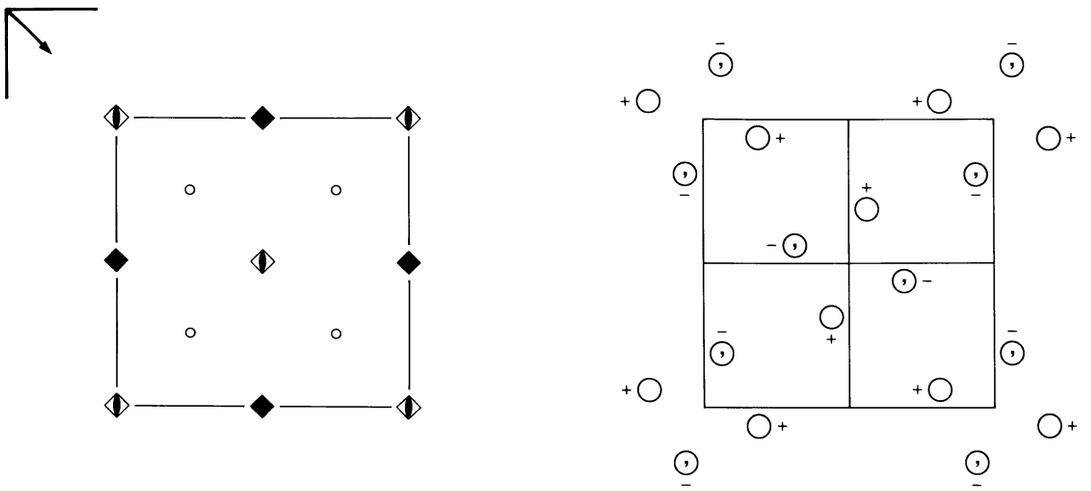
$P4/n$ C_{4h}^3 $4/m$ Tetragonal

No. 85 $P4/n$ Patterson symmetry $P4/m$

ORIGIN CHOICE 1



Origin at $\bar{4}$ on n, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,\frac{1}{2},z$	(4) 4^- $\frac{1}{2},0,z$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $\bar{4}^+$ $0,0,z$; $0,0,0$	(8) $\bar{4}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y},x,\bar{z}$	$h00$: $h=2n$
							Special: as above, plus
4	f	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl: $h+k=2n$
4	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl: $h,k=2n$
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h,k=2n$
2	c	4 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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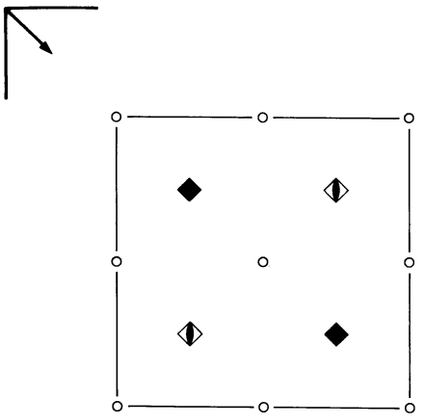
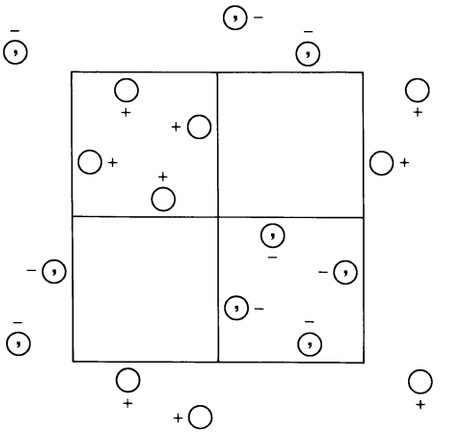
Tetragonal $4/m$ C_{4h}^3 $P4/n$

Patterson symmetry $P4/m$ $P4/n$ No. 85

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{4}$; $-\frac{1}{4}\le y\le\frac{1}{4}$; $0\le z\le\frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 4^+ $\frac{1}{4},\frac{1}{4},z$	(4) 4^- $\frac{1}{4},\frac{1}{4},z$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$	(8) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},\bar{x},\bar{z}$	(8) $\bar{y},x+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
							Special: as above, plus
4	f	2 . .	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	hkl: $h+k=2n$
4	e	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h,k=2n$
4	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h,k=2n$
2	c	4 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	b	$\bar{4}$ . .	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}$ . .	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

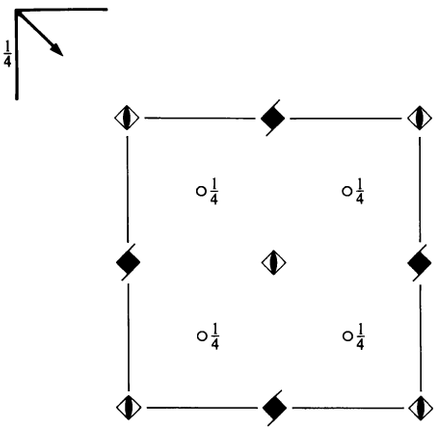
Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

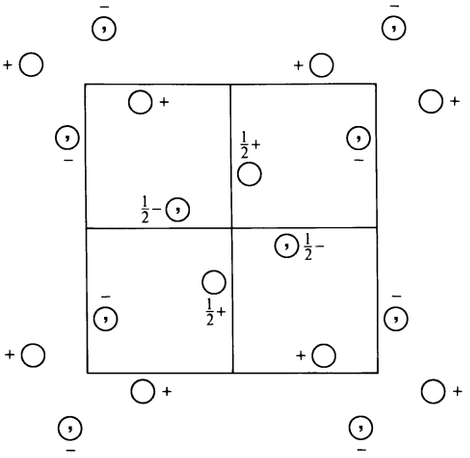
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$P4_2/n$ C_{4h}^4 $4/m$ Tetragonal

No. 86 $P4_2/n$ Patterson symmetry $P4/m$

ORIGIN CHOICE 1





Origin at $\bar{4}$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ (6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$ (7) $\bar{4}^+$ $0,0,z$; $0,0,0$ (8) $\bar{4}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y},x,\bar{z}$	
							Special: as above, plus
4	f	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl: $h+k+l=2n$
4	e	2 . .	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$
4	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$
4	c	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

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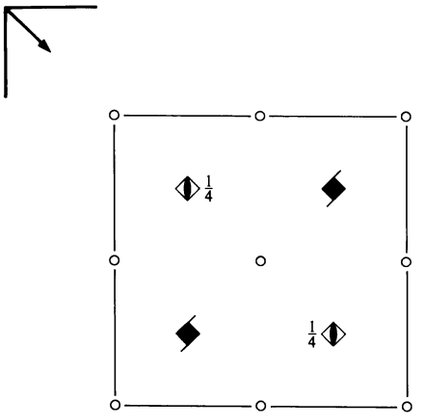
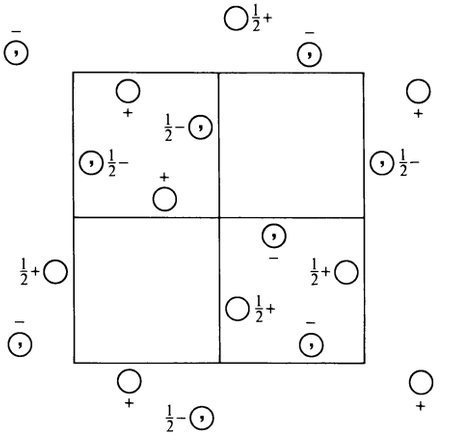
Tetragonal $4/m$ C_{4h}^4 $P4_2/n$

Patterson symmetry $P4/m$ $P4_2/n$ No. 86

ORIGIN CHOICE 2





Origin at $\bar{1}$ on n, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},-\frac{1}{4},z$
(5) $\bar{1}$ $0,0,0$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(7) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z;$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(8) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z;$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$ (7) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$hk0$: $h+k=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
4	f	2 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
4	e	2 . .	$\frac{3}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl: $h+k,h+l,k+l=2n$
4	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
2	b	$\bar{4}$ . .	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$			hkl: $h+k+l=2n$
2	a	$\bar{4}$ . .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

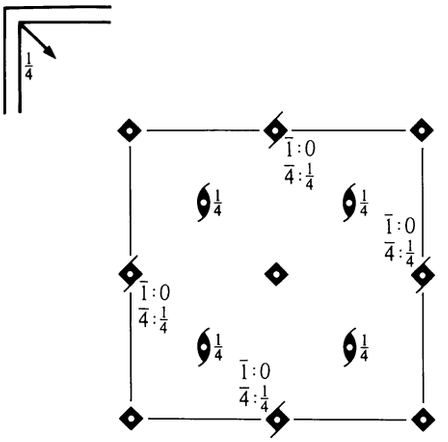
Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

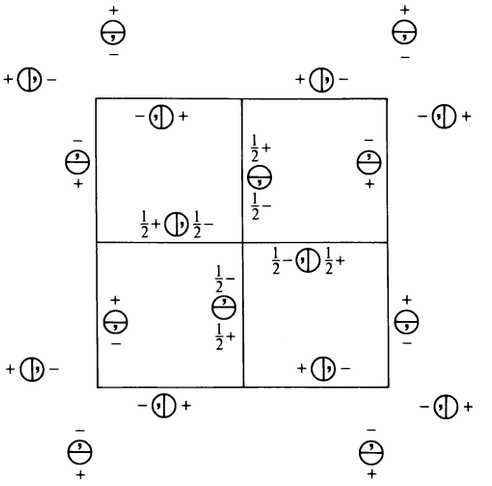
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

International Tables for Crystallography (2016). Vol. A, Space group 87, pp. 398–399.

$I4/m$ C_{4h}^5 $4/m$ Tetragonal

No. 87 $I4/m$ Patterson symmetry $I4/m$





Origin at centre $(4/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) $\bar{1}$ $0,0,0$	(6) m $x,y,0$	(7) $\bar{4}^+$ $0,0,z$; $0,0,0$	(8) $\bar{4}^-$ $0,0,z$; $0,0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(8) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			General:
16	i	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	h	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
8	g	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$
8	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl: $k,l=2n$
4	e	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	$\bar{4}$ . .	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl: $l=2n$
4	c	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $l=2n$
2	b	$4/m$ . .	$0,0,\frac{1}{2}$				no extra conditions
2	a	$4/m$ . .	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

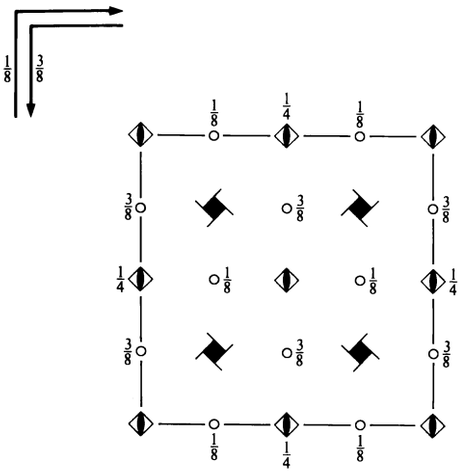
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

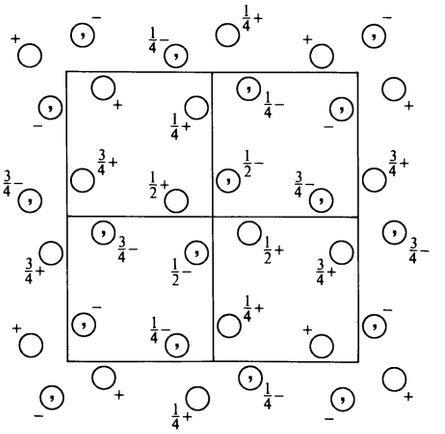
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$I4_1/a$ C_{4h}^6 $4/m$ Tetragonal

No. 88 $I4_1/a$ Patterson symmetry $I4/m$

ORIGIN CHOICE 1





Origin at $\bar{4}$, at $0,-\frac{1}{4},-\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) $\bar{1}$ $0,\frac{1}{4},\frac{1}{8}$	(6) a $x,y,\frac{3}{8}$	(7) $\bar{4}^+$ $0,0,z$; $0,0,0$	(8) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) $\bar{1}$ $\frac{1}{4},0,\frac{3}{8}$	(6) b $x,y,\frac{1}{8}$	(7) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(8) $\bar{4}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$		$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		Reflection conditions
							General:
16	f	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl: $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
			(5) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(7) $y,\bar{x},\bar{z}$	(8) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	
							Special: as above, plus
8	e	2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$0,\frac{1}{2},\bar{z}+\frac{1}{4}$	$0,0,\bar{z}$	hkl: $l=2n+1$ or $2h+l=4n$
8	d	$\bar{1}$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$	hkl: $l=2n+1$ or $h,k=2n$, $h+k+l=4n$
8	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$	
4	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}$ . .	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			

Symmetry of special projections

Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $p2mg$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{1}{8}$

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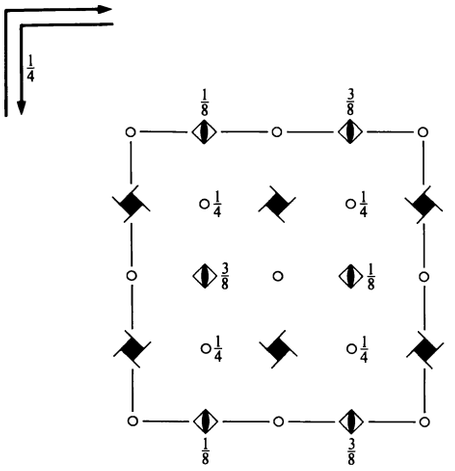
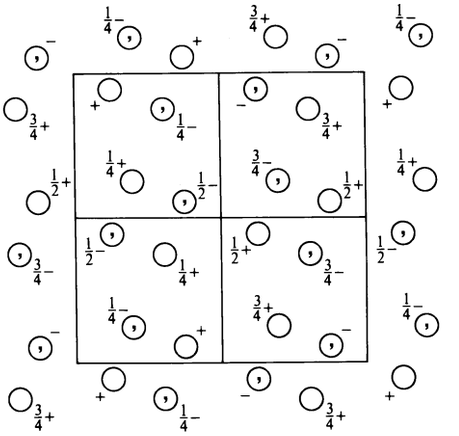




Origin at $\bar{1}$ on glide plane b, at $0, \frac{1}{4}, \frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{4}; \quad 0 \le y \le \frac{1}{4}; \quad 0 \le z \le 1$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{3}{4},0,z$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z;$ $\frac{1}{2},\frac{1}{4},\frac{3}{8}$	(8) $\bar{4}^-$ $0,\frac{1}{4},z;$ $0,\frac{1}{4},\frac{1}{8}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},0,z$
(5) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(6) b $x,y,0$	(7) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z;$ $\frac{1}{2},-\frac{1}{4},\frac{1}{8}$	(8) $\bar{4}^-$ $0,\frac{3}{4},z;$ $0,\frac{3}{4},\frac{3}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
						General:
16 f 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{3}{4},x+\frac{1}{4},z+\frac{1}{4}$	(4) $y+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$		hkl: $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
	(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(8) $\bar{y}+\frac{1}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$		
						Special: as above, plus
8 e 2 . .	$0,\frac{1}{4},z$	$\frac{1}{2},\frac{1}{4},z+\frac{1}{4}$	$0,\frac{3}{4},\bar{z}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{3}{4}$		hkl: $l=2n+1$ or $2h+l=4n$
8 d $\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	}	hkl: $l=2n+1$ or $h,k=2n, \quad h+k+l=4n$
8 c $\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	}	
4 b $\bar{4}$ . .	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{7}{8}$			}	hkl: $l=2n+1$ or $2h+l=4n$
4 a $\bar{4}$ . .	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{3}{8}$			}	

Symmetry of special projections

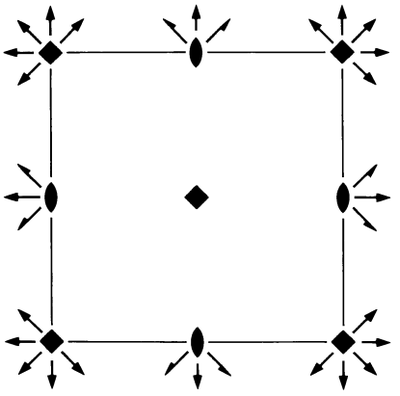
Along [001] $p4$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4},0,z$

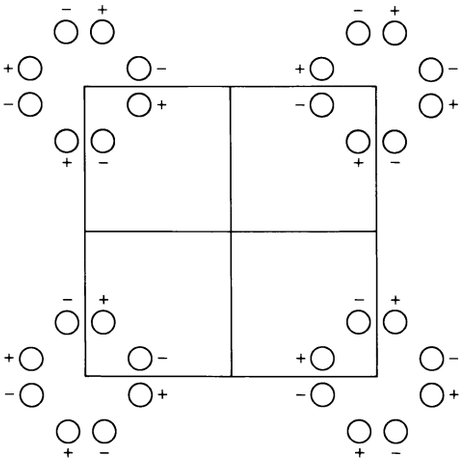
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mg$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P422$ D_4^1 422 Tetragonal

No. 89 $P422$ Patterson symmetry $P4/mmm$





Origin at 422

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	p	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special:
4	o	. 2 .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	n	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
4	m	. 2 .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	l	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	k	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	no extra conditions
4	j	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $h+k=2n$
2	h	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	2 2 2 .	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	e	2 2 2 .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl: $h+k=2n$
1	d	4 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	4 2 2	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	4 2 2	$0,0,\frac{1}{2}$				no extra conditions
1	a	4 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

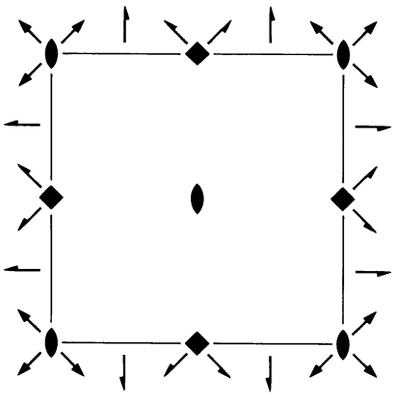
Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

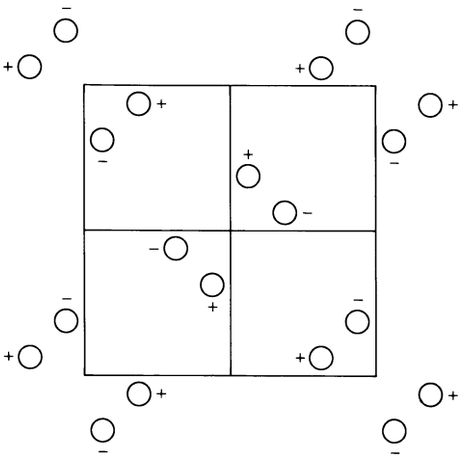
Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$P4_12_12$ D_4^2 422 Tetragonal

No. 90 $P4_12_12$ Patterson symmetry $P4/mmm$





Origin at 222 at 212

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,\frac{1}{2},z$	(4) 4^- $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$ (7) $y,x,\bar{z}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$ (8) $\bar{y},\bar{x},\bar{z}$	$h00$: $h=2n$
							Special: as above, plus
4	f	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0kl$: $k=2n$
4	e	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$0kl$: $k=2n$
4	d	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl: $h+k=2n$
2	c	4 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	b	2 . 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	2 . 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

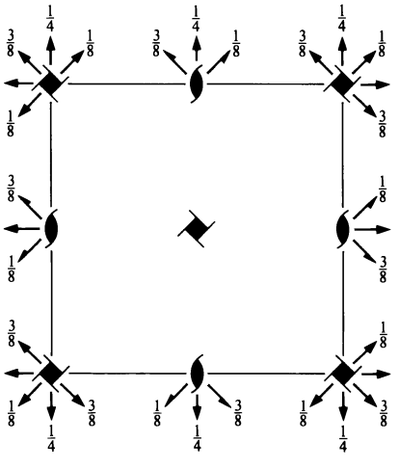
Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

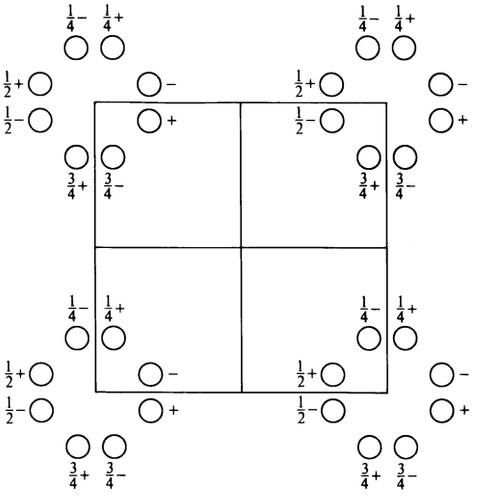
Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$P4_122$ D_4^3 422 Tetragonal

No. 91 $P4_122$ Patterson symmetry $P4/mmm$





Origin on $2\,[0\,1\,0]$ at $4_1\,(1,2)\,1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{1}{4})$ $0,0,z$ (4) $4^-(0,0,\frac{3}{4})$ $0,0,z$
(5) 2 $0,y,0$ (6) 2 $x,0,\frac{1}{4}$ (7) 2 $x,x,\frac{3}{8}$ (8) 2 $x,\bar{x},\frac{1}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{1}{4}$	(4) $y,\bar{x},z+\frac{3}{4}$	$00l$: $l=4n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{3}{4}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{4}$	
							Special: as above, plus
4	c	. . 2	$x,x,\frac{3}{8}$	$\bar{x},\bar{x},\frac{7}{8}$	$\bar{x},x,\frac{5}{8}$	$x,\bar{x},\frac{1}{8}$	$0kl$: $l=2n+1$ or $l=4n$
4	b	. 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},\frac{1}{2}$	$\bar{y},\frac{1}{2},\frac{1}{4}$	$y,\frac{1}{2},\frac{3}{4}$	hhl: $l=2n+1$ or $l=4n$
4	a	. 2 .	$0,y,0$	$0,\bar{y},\frac{1}{2}$	$\bar{y},0,\frac{1}{4}$	$y,0,\frac{3}{4}$	hhl: $l=2n+1$ or $l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p2gm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{3}{8}$

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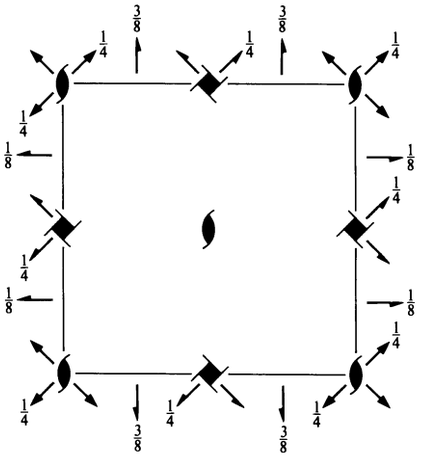
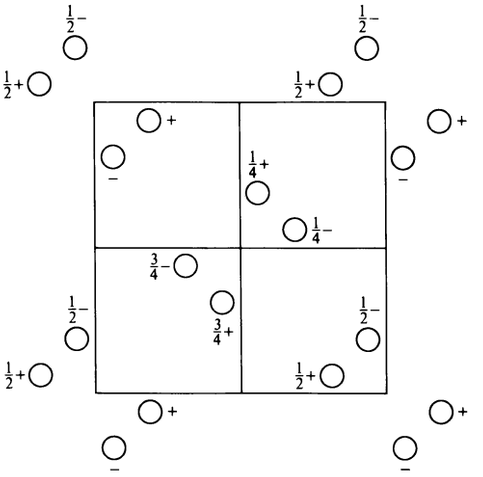
Tetragonal 422 D_4^4 $P4_12_12$

Patterson symmetry $P4/mmm$ $P4_12_12$ No. 92





Origin on $2\,[1\,1\,0]$ at $2_1\,1\,(1,2)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{1}{4})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{8}$ (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{3}{8}$ (7) 2 $x,x,0$ (8) 2 $x,\bar{x},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8	*b* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	$00l$: $l=4n$ $h00$: $h=2n$
		(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{4}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{3}{4}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	
						Special: as above, plus
4	*a* . . 2	$x,x,0$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$0kl$: $l=2n+1$ or $2k+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $p2gg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{3}{8}$

Along [110] $p2gm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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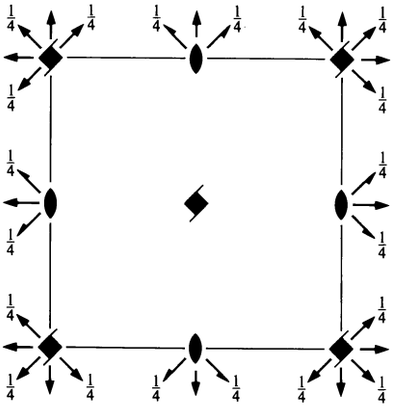
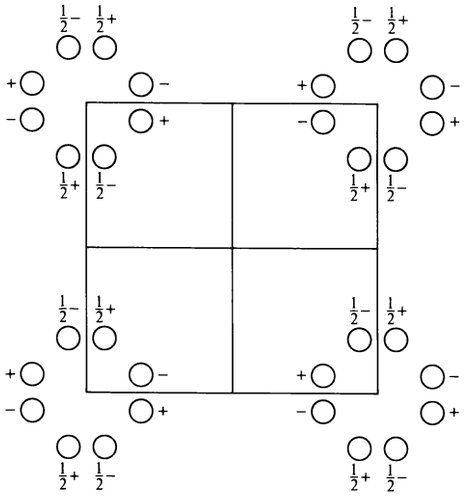
$P4_222$ D_4^5 422 Tetragonal

No. 93 $P4_222$ Patterson symmetry $P4/mmm$





Origin at 222 at $4_2$21

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) $4^+(0,0,\frac{1}{2})$ $0,0,z$
(4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) 2 $0,y,0$
(6) 2 $x,0,0$
(7) 2 $x,x,\frac{1}{4}$
(8) 2 $x,\bar{x},\frac{1}{4}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	p	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z+\frac{1}{2}$ (7) $y,x,\bar{z}+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
4	o	. . 2	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$0kl$: $l=2n$
4	n	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	$0kl$: $l=2n$
4	m	. 2 .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	hhl: $l=2n$
4	l	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,0$	$0,\bar{x},0$	hhl: $l=2n$
4	k	. 2 .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	hhl: $l=2n$
4	j	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	hhl: $l=2n$
4	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
4	h	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	g	2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
2	f	2 . 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	e	2 . 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$
2	d	2 2 2 .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl: $h+k+l=2n$
2	c	2 2 2 .	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	b	2 2 2 .	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	a	2 2 2 .	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

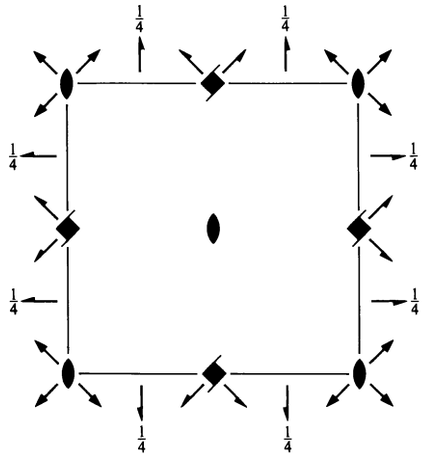
Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

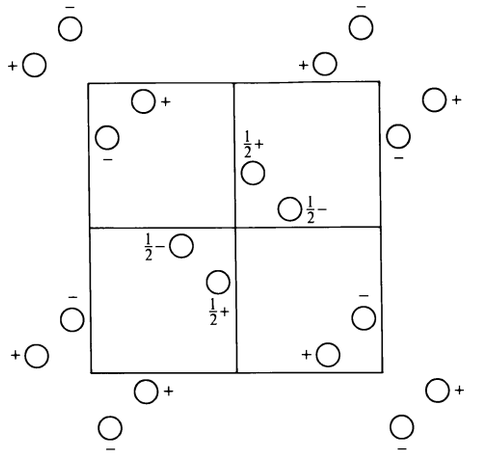
Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

$P4_22_12$ D_4^6 422 Tetragonal

No. 94 $P4_22_12$ Patterson symmetry $P4/mmm$





Origin at 222 at 212

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$
(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$
(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(7) 2 $x,x,0$
(8) 2 $x,\bar{x},0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$00l$: $l=2n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	
							Special: as above, plus
4	f	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$0kl$: $k+l=2n$
4	e	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0kl$: $k+l=2n$
4	d	2 . .	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$ $hk0$: $h+k=2n$
4	c	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl: $h+k+l=2n$
2	b	2 . 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	2 . 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

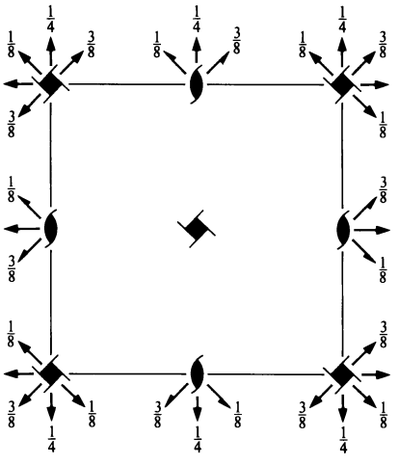
Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

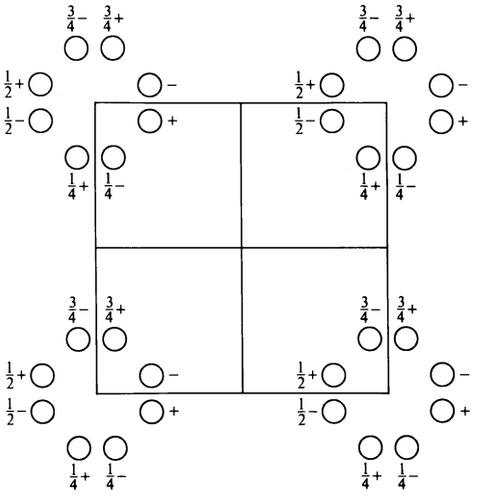
Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$P4_322$ D_4^7 422 Tetragonal

No. 95 $P4_322$ Patterson symmetry $P4/mmm$





Origin on $2\,[0\,1\,0]$ at $4_3\,(1,2)\,1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{3}{4})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{4})$ $0,0,z$
(5) 2 $0,y,0$ (6) 2 $x,0,\frac{1}{4}$ (7) 2 $x,x,\frac{1}{8}$ (8) 2 $x,\bar{x},\frac{3}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
8	*d* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y},x,z+\frac{3}{4}$	(4) $y,\bar{x},z+\frac{1}{4}$	$00l$: $l=4n$
		(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{4}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{3}{4}$	
						Special: as above, plus
4	*c* . . 2	$x,x,\frac{5}{8}$	$\bar{x},\bar{x},\frac{1}{8}$	$\bar{x},x,\frac{3}{8}$	$x,\bar{x},\frac{7}{8}$	$0kl$: $l=2n+1$ or $l=4n$
4	*b* . 2 .	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},\frac{1}{2}$	$\bar{y},\frac{1}{2},\frac{3}{4}$	$y,\frac{1}{2},\frac{1}{4}$	hhl: $l=2n+1$ or $l=4n$
4	*a* . 2 .	$0,y,0$	$0,\bar{y},\frac{1}{2}$	$\bar{y},0,\frac{3}{4}$	$y,0,\frac{1}{4}$	hhl: $l=2n+1$ or $l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p2gm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{8}$

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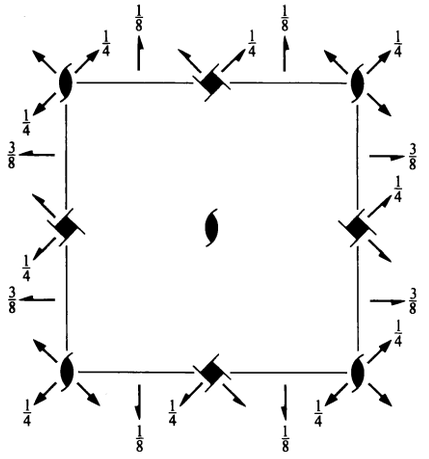
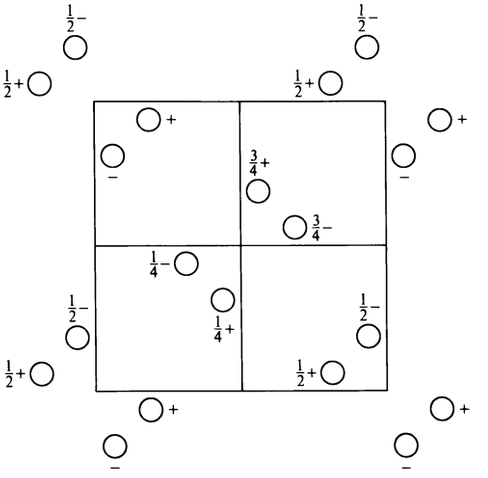
Tetragonal 422 D_4^8 $P4_32_12$

Patterson symmetry $P4/mmm$ $P4_32_12$ No. 96





Origin on $2\,[1\,1\,0]$ at $2_1\,1\,(1,2)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{8}$

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{3}{4})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{3}{8}$ (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{8}$ (7) 2 $x,x,0$ (8) 2 $x,\bar{x},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 b 1	(1) x,y,z	(2) $\bar{x},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{3}{4}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	$00l$: $l=4n$
	(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$h00$: $h=2n$
					Special: as above, plus
4 a . . 2	$x,x,0$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	$0kl$: $l=2n+1$ or $2k+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $p2gg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{8}$

Along [110] $p2gm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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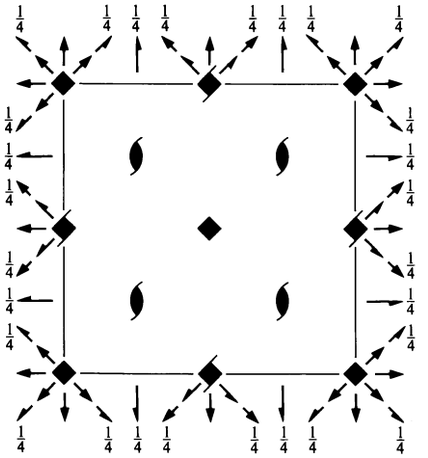
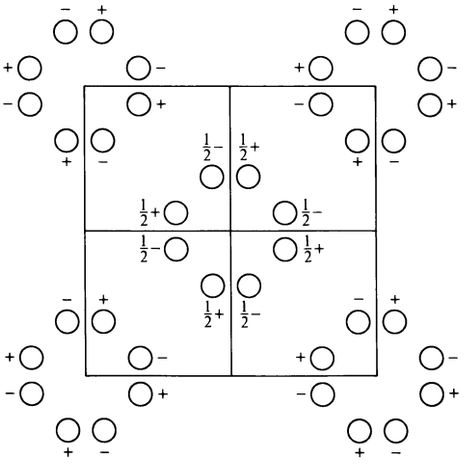
$I422$ D_4^9 422 Tetragonal

No. 97 $I422$ Patterson symmetry $I4/mmm$





Origin at 422

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	*k*	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	*j*	. . 2	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	$0kl$: $k=2n$
8	*i*	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
8	*h*	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
8	*g*	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
8	*f*	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$
4	*e*	4 . .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	*d*	2 . 2 2	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl: $l=2n$
4	*c*	2 2 2 .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $l=2n$
2	*b*	4 2 2	$0,0,\frac{1}{2}$				no extra conditions
2	*a*	4 2 2	$0,0,0$				no extra conditions

Symmetry of special projections

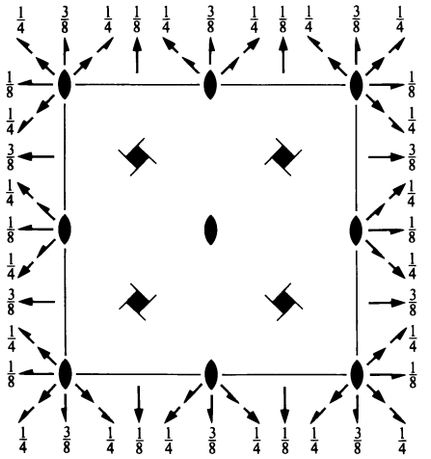
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

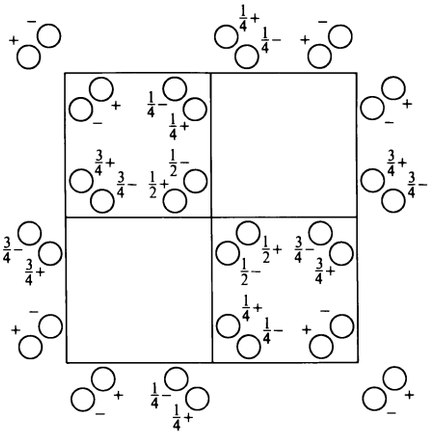
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$I4_122$ D_4^{10} 422 Tetragonal

No. 98 $I4_122$ Patterson symmetry $I4/mmm$





Origin at 222 at 212

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,\frac{3}{8}$	(6) 2 $x,\frac{1}{4},\frac{1}{8}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{8}$	(6) $2(\frac{1}{2},0,0)$ $x,0,\frac{3}{8}$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	Coordinates $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
							General:
16	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=4n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}$	
							Special: as above, plus
8	f	.2.	$x,\frac{1}{4},\frac{1}{8}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},\bar{x},\frac{7}{8}$	hhl: $l=4n$
8	e	..2	$\bar{x},x,0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	$0kl$: $k=2n+1$ or $l=4n$
8	d	..2	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$0kl$: $k=2n+1$ or $l=4n$
8	c	2..	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $l=2n+1$ or $2h+l=4n$
4	b	2.22	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n+1$ or $2h+l=4n$
4	a	2.22	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			hkl: $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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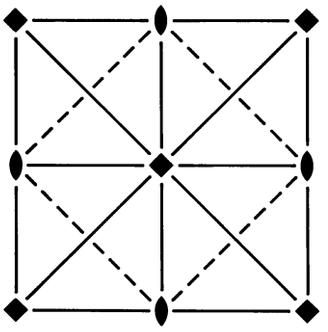
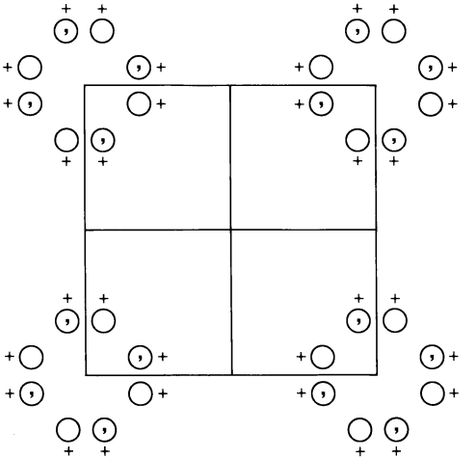
Tetragonal $4mm$ C_{4v}^{1} $P4mm$

Patterson symmetry $P4/mmm$ $P4mm$ No. 99





Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$
(5) m $x,0,z$ (6) m $0,y,z$ (7) m $x,\bar{x},z$ (8) m x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	g	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) y,x,z	no conditions
							Special:
4	f	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z$	$\frac{1}{2},\bar{x},z$	no extra conditions
4	e	. m .	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
4	d	. . m	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
2	c	2 m m .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl: $h+k=2n$
1	b	4 m m	$\frac{1}{2},\frac{1}{2},z$				no extra conditions
1	a	4 m m	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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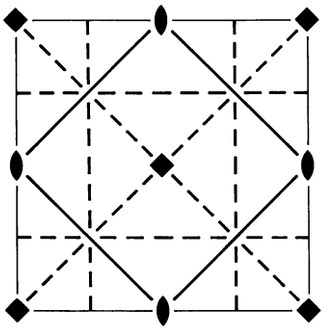
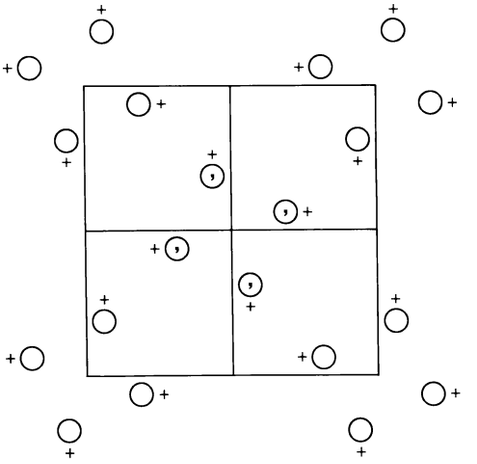
$P4bm$ C_{4v}^2 $4mm$ Tetragonal

No. 100 $P4bm$ Patterson symmetry $P4/mmm$





Origin on $4\,1\,g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) m $x+\frac{1}{2},\bar{x},z$	(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$	$h00$: $h=2n$
							Special: as above, plus
4	c	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
2	b	$2\,.\,mm$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl: $h+k=2n$
2	a	$4\,..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p\,4\,g\,m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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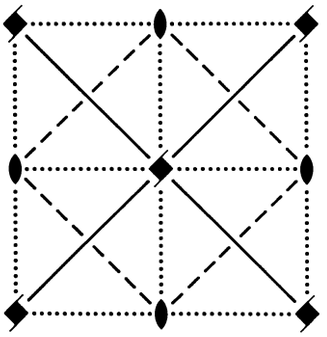
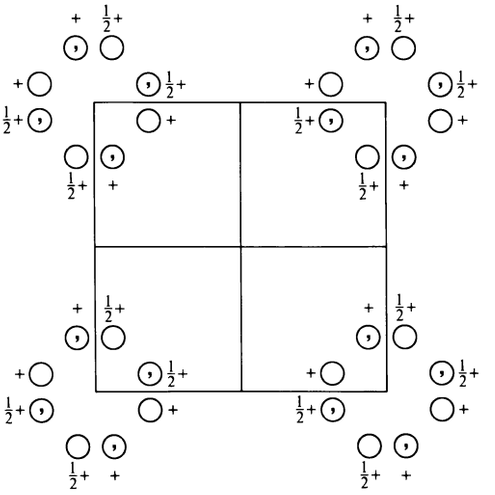
Tetragonal $4mm$ C_{4v}^3 $P4_2cm$

Patterson symmetry $P4/mmm$ $P4_2cm$ No. 101





Origin on $2mm$ on 4_2cm

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) c $x,0,z$ (6) c $0,y,z$ (7) m $x,\bar{x},z$ (8) m x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$0kl$: $l=2n$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	$00l$: $l=2n$
							Special: as above, plus
4	d	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$x,\bar{x},z+\frac{1}{2}$	no extra conditions
4	c	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z$	hkl: $h+k,l=2n$
2	b	$2.mm$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $l=2n$
2	a	$2.mm$	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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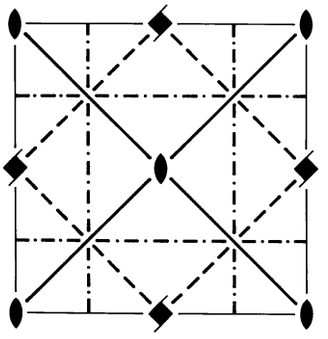
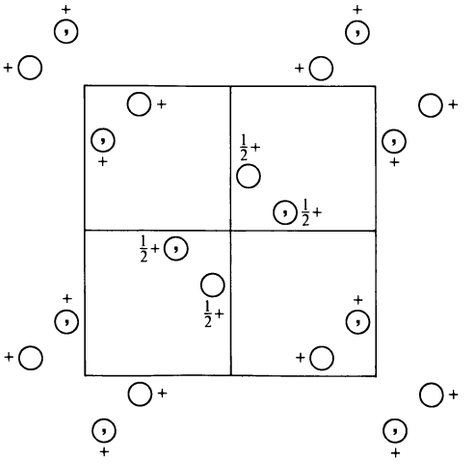
$P4_2nm$ C_{4v}^4 $4mm$ Tetragonal

No. 102 $P4_2nm$ Patterson symmetry $P4/mmm$





Origin on $2mm$ on $2\,1\,m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$ (7) m $x,\bar{x},z$ (8) m x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	
							Special: as above, plus
4	c	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
4	b	$2..$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$	hkl: $h+k,l=2n$
2	a	$2.mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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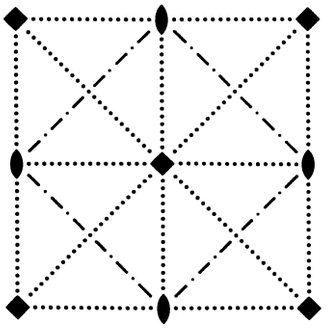
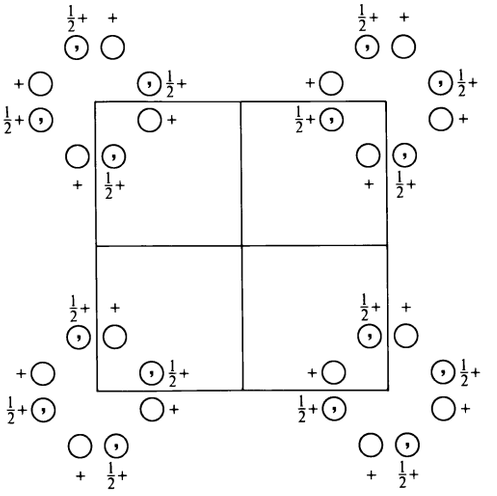
Tetragonal $4mm$ C_{4v}^5 $P4cc$

Patterson symmetry $P4/mmm$ $P4cc$ No. 103





Origin on $4c\,c$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$
(5) c $x,0,z$ (6) c $0,y,z$ (7) c $x,\bar{x},z$ (8) c x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 d 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $l=2n$
	(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$	hhl: $l=2n$
					$00l$: $l=2n$
					Special: as above, plus
4 c 2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl: $h+k,l=2n$
2 b 4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $l=2n$
2 a 4 . .	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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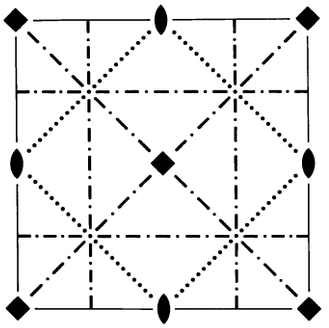
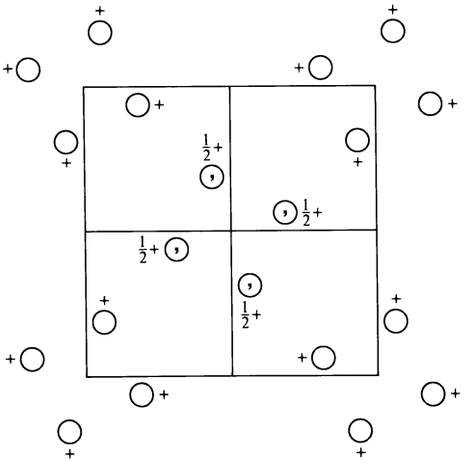
$P4nc$ C_{4v}^{6} $4mm$ Tetragonal

No. 104 $P4nc$ Patterson symmetry $P4/mmm$





Origin on $4\,1\,n$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) 4^+ $0,0,z$ (4) 4^- $0,0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$ (7) c $x+\frac{1}{2},\bar{x},z$ (8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	
							Special: as above, plus
4	b	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k,l=2n$
2	a	4 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p\,4\,g\,m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $c\,1\,m\,1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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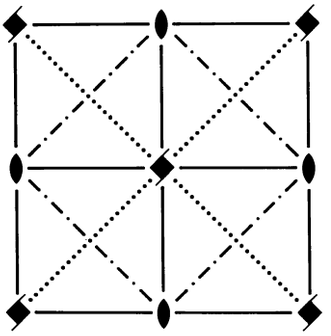
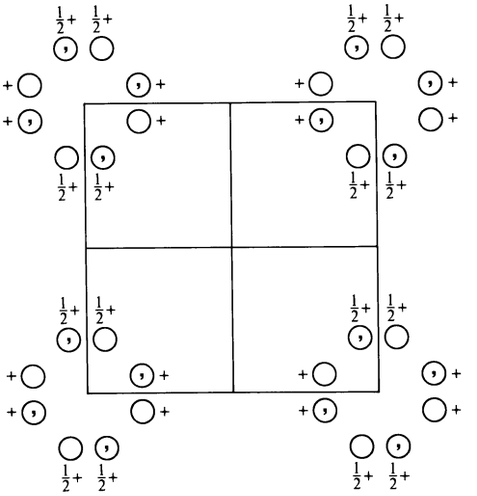
Tetragonal $4mm$ C_{4v}^{7} $P4_2mc$

Patterson symmetry $P4/mmm$ $P4_2mc$ No. 105





Origin on $2mm$ on 4_2mc

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) m $x,0,z$ (6) m $0,y,z$ (7) c $x,\bar{x},z$ (8) c x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	hhl: $l=2n$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
4	e	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},x,z+\frac{1}{2}$	$\frac{1}{2},\bar{x},z+\frac{1}{2}$	no extra conditions
4	d	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z+\frac{1}{2}$	$0,\bar{x},z+\frac{1}{2}$	no extra conditions
2	c	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$			hkl: $h+k+l=2n$
2	b	$2mm.$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			hkl: $l=2n$
2	a	$2mm.$	$0,0,z$	$0,0,z+\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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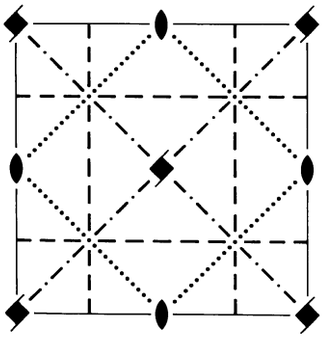
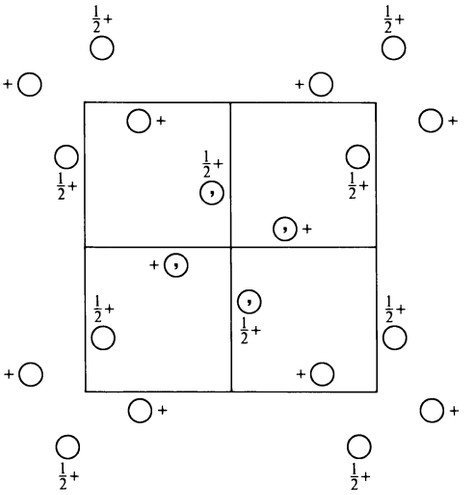
$P4_2bc$ C_{4v}^8 $4mm$ Tetragonal

No. 106 $P4_2bc$ Patterson symmetry $P4/mmm$





Origin on 2 on $4_2\,1\,n$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $4^+(0,0,\frac{1}{2})$ $0,0,z$ (4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) a $x,\frac{1}{4},z$ (6) b $\frac{1}{4},y,z$ (7) c $x+\frac{1}{2},\bar{x},z$ (8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$0kl$: $k=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	
							Special: as above, plus
4	b	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k,l=2n$
4	a	2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k,l=2n$

Symmetry of special projections

Along [001] $p\,4\,g\,m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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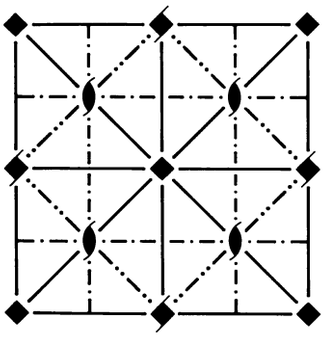
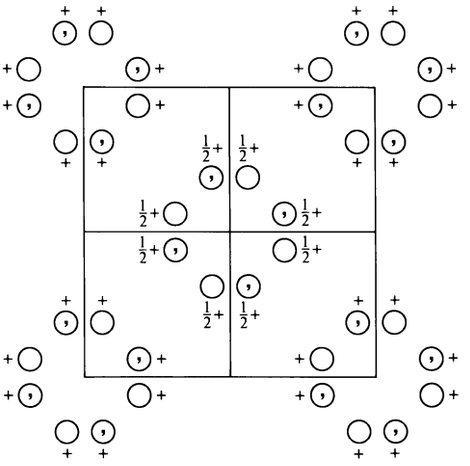
Tetragonal $4mm$ C_{4v}^{9} $I4mm$

Patterson symmetry $I4/mmm$ $I4mm$ No. 107





Origin on $4mm$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) m $x,0,z$	(6) m $0,y,z$	(7) m $x,\bar{x},z$	(8) m x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(7) c $x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	hkl: $h+k+l=2n$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	$hk0$: $h+k=2n$
							$0kl$: $k+l=2n$
							hhl: $l=2n$
							$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
8	d	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
8	c	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
4	b	$2\,m\,m.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			hkl: $l=2n$
2	a	$4\,m\,m$	$0,0,z$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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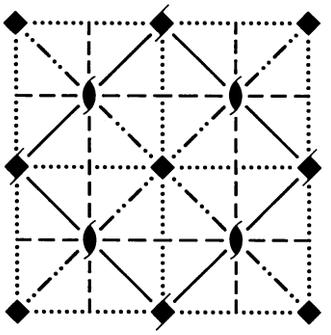
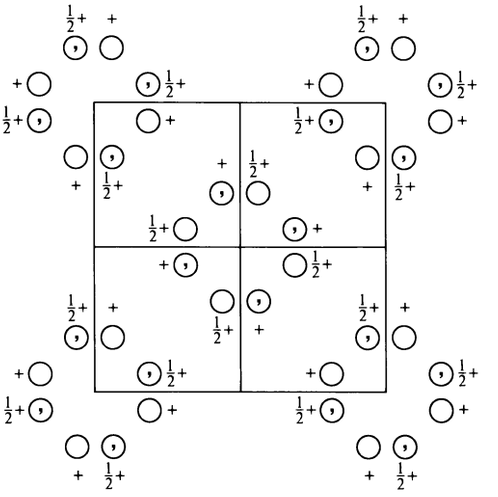
$I4cm$ C_{4v}^{10} $4mm$ Tetragonal

No. 108 $I4cm$ Patterson symmetry $I4/mmm$





Origin on $4c\,e$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad y \le \frac{1}{2} - x$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) c $x,0,z$	(6) c $0,y,z$	(7) c $x,\bar{x},z$	(8) c x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) m $x+\frac{1}{2},\bar{x},z$	(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
						General:
16	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$
						hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k,l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
						Special: as above, plus
8	c	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$
						no extra conditions
4	b	$2\,.\,mm$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$		hkl: $l=2n$
4	a	$4\,..$	$0,0,z$	$0,0,z+\frac{1}{2}$		hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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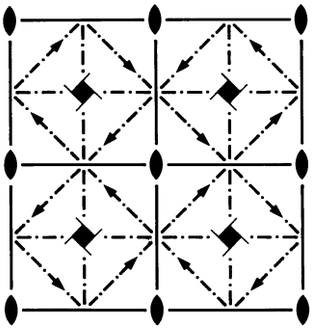
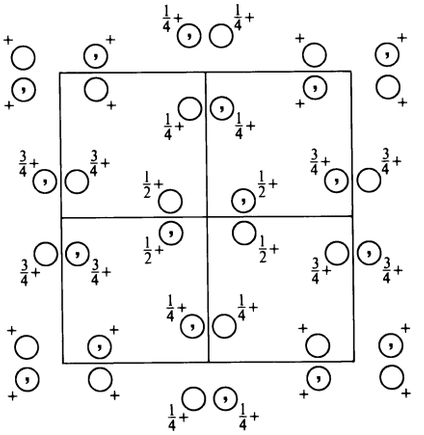
Tetragonal $4mm$ C_{4v}^{11} $I4_1md$

Patterson symmetry $I4/mmm$ $I4_1md$ No. 109





Origin on $2mm$ on $2m1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) m $x,0,z$	(6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(6) m $0,y,z$	(7) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
						General:
16 c 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$		hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $2h+l=4n$ $00l$: $l=4n$ $h\bar{h}0$: $h=2n$
	(5) $x,\bar{y},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{1}{4}$	(8) $y+\frac{1}{2},x,z+\frac{3}{4}$		$h0\bar{0}$: $h=2n$
						Special: as above, plus
8 b $.m.$	$0,y,z$	$\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$\bar{y},\frac{1}{2},z+\frac{1}{4}$	$y+\frac{1}{2},0,z+\frac{3}{4}$		no extra conditions
4 a $2mm.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$				hkl: $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $c1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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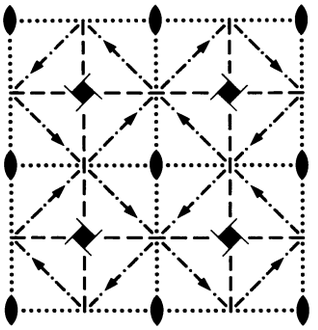
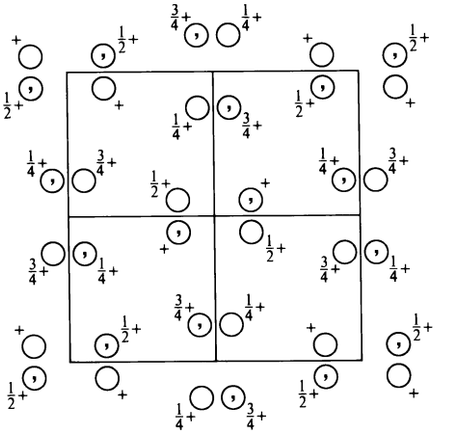
$I4_1cd$ C_{4v}^{12} $4mm$ Tetragonal

No. 110 $I4_1cd$ Patterson symmetry $I4/mmm$





Origin on $2c\,1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) c $x,0,z$	(6) b $\frac{1}{4},y,z$	(7) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) a $x,\frac{1}{4},z$	(6) c $0,y,z$	(7) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x-\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
					General:
16 b 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl: $h+k+l=2n$
	(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(8) $y+\frac{1}{2},x,z+\frac{1}{4}$	$hk0$: $h+k=2n$
					$0kl$: $k,l=2n$
					hhl: $2h+l=4n$
					$00l$: $l=4n$
					$h\bar{h}00$: $h=2n$
					$h\bar{h}0$: $h=2n$
					Special: as above, plus
8 a 2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$0,0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{3}{4}$	hkl: $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $c1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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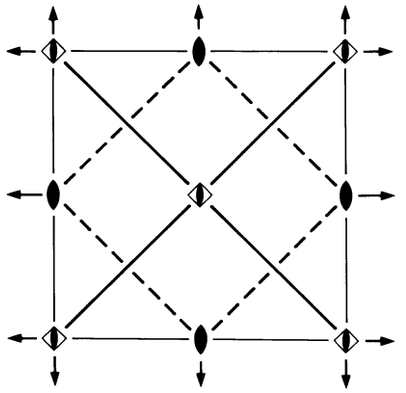
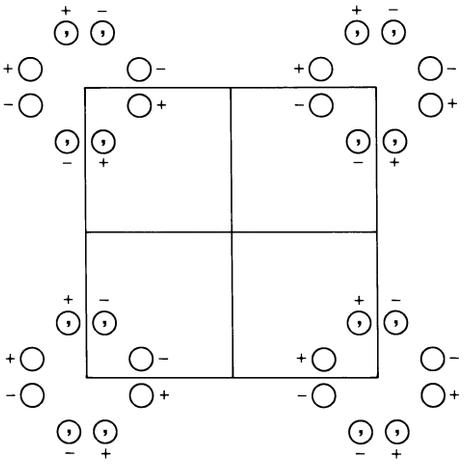
Tetragonal $\bar{4}2m$ D_{2d}^1 $P\bar{4}2m$

Patterson symmetry $P4/mmm$ $P\bar{4}2m$ No. 111





Origin at $\bar{4}2m$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le 1; \quad x \le y$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ (4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) 2 $0,y,0$ (6) 2 $x,0,0$ (7) m $x,\bar{x},z$ (8) m x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	o	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y},\bar{x},z$	(4) $\bar{y},x,\bar{z}$ (8) y,x,z	no conditions
							Special:
4	n	$..m$	x,x,z	$\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	no extra conditions
4	m	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl: $h+k=2n$
4	l	$.2.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},\bar{x},0$	$\frac{1}{2},x,0$	no extra conditions
4	k	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	no extra conditions
4	j	$.2.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	no extra conditions
4	i	$.2.$	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	no extra conditions
2	h	$2.mm$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	$2.mm$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	$222.$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	e	$222.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$			hkl: $h+k=2n$
1	d	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	c	$\bar{4}2m$	$0,0,\frac{1}{2}$				no extra conditions
1	b	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	a	$\bar{4}2m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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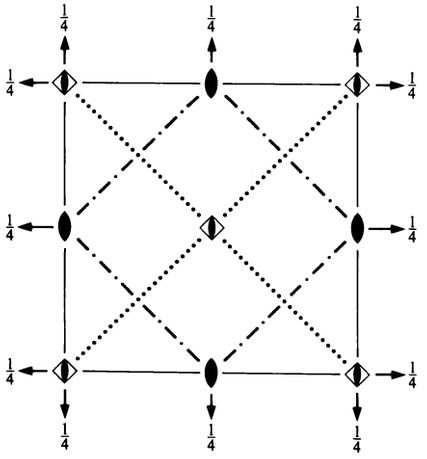
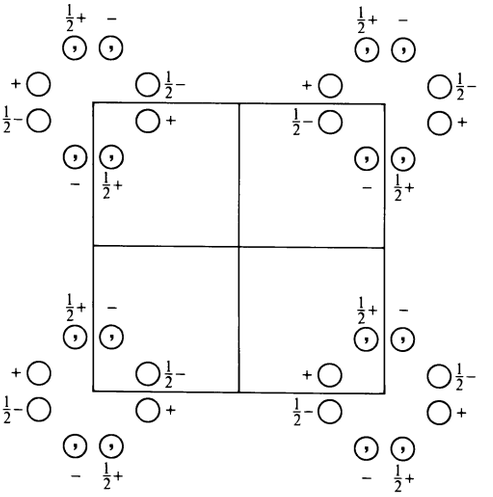
$P\bar{4}2c$ D_{2d}^2 $\bar{4}2m$ Tetragonal

No. 112 $P\bar{4}2c$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}1c$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ (4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) 2 $0,y,\frac{1}{4}$ (6) 2 $x,0,\frac{1}{4}$ (7) c $x,\bar{x},z$ (8) c x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	hhl: $l=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $y,x,z+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
4	m	2..	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	l	2..	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
4	k	2..	$0,0,z$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
4	j	.2.	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$y,0,\frac{3}{4}$	$\bar{y},0,\frac{3}{4}$	no extra conditions
4	i	.2.	$x,\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\bar{x},\frac{3}{4}$	$\frac{1}{2},x,\frac{3}{4}$	no extra conditions
4	h	.2.	$\frac{1}{2},y,\frac{1}{4}$	$\frac{1}{2},\bar{y},\frac{1}{4}$	$y,\frac{1}{2},\frac{3}{4}$	$\bar{y},\frac{1}{2},\frac{3}{4}$	no extra conditions
4	g	.2.	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$	no extra conditions
2	f	$\bar{4}$..	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	e	$\bar{4}$..	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
2	d	222.	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl: $h+k+l=2n$
2	c	222.	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	b	222.	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $h+k+l=2n$
2	a	222.	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{4}$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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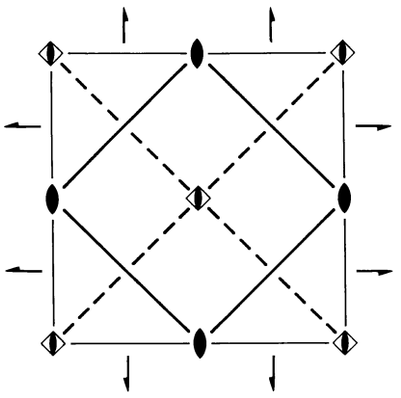
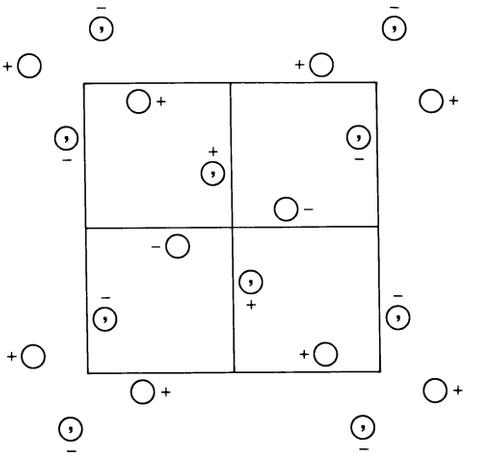
Tetragonal $\bar{4}2m$ D_{2d}^3 $P\bar{4}2_1m$

Patterson symmetry $P4/mmm$ $P\bar{4}2_1m$ No. 113





Origin at $\bar{4}1g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) m $x+\frac{1}{2},\bar{x},z$	(8) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	f	1	(1) x,y,z (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(3) $y,\bar{x},\bar{z}$ (7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(4) $\bar{y},x,\bar{z}$ (8) $y+\frac{1}{2},x+\frac{1}{2},z$	$h00$: $h=2n$
							Special: as above, plus
4	e	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$x+\frac{1}{2},\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x,\bar{z}$	no extra conditions
4	d	$2..$	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl: $h+k=2n$
2	c	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	b	$\bar{4}..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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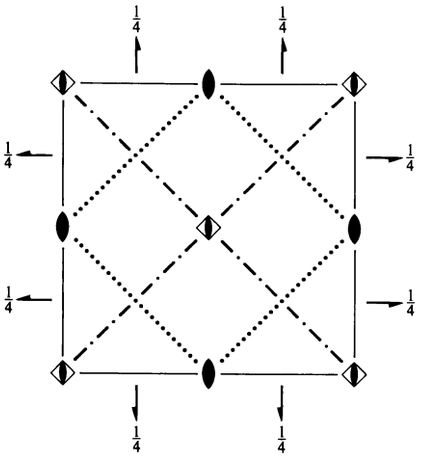
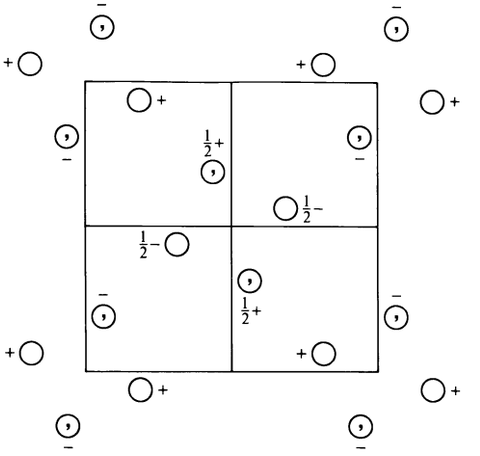
$P\bar{4}2_1c$ D_{2d}^4 $\bar{4}2m$ Tetragonal

No. 114 $P\bar{4}2_1c$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}1n$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ (4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$ (7) c $x+\frac{1}{2},\bar{x},z$ (8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(8) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	
							Special: as above, plus
4	d	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$ $hk0$: $h+k=2n$
4	c	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k+l=2n$
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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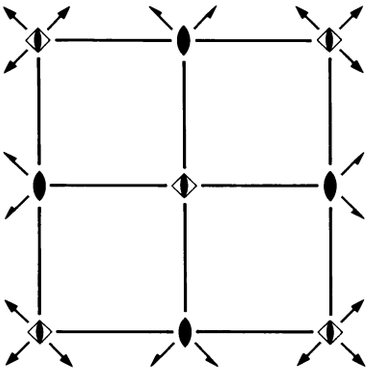
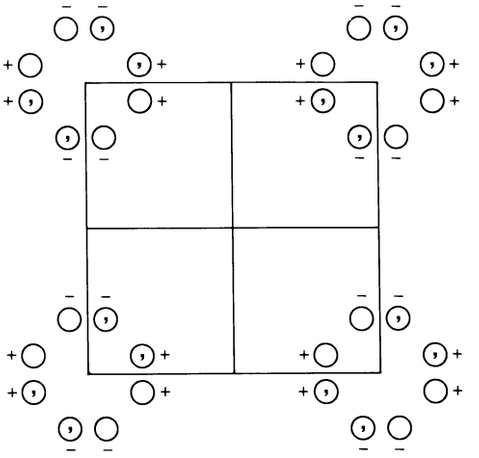
Tetragonal $\bar{4}m2$ D_{2d}^5 $P\bar{4}m2$

Patterson symmetry $P4/mmm$ $P\bar{4}m2$ No. 115





Origin at $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ (4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) m $x,0,z$ (6) m $0,y,z$ (7) 2 $x,x,0$ (8) 2 $x,\bar{x},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	l	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$	no conditions
							Special:
4	k	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\frac{1}{2},\bar{x},\bar{z}$	$\frac{1}{2},x,\bar{z}$	no extra conditions
4	j	. m .	$x,0,z$	$\bar{x},0,z$	$0,\bar{x},\bar{z}$	$0,x,\bar{z}$	no extra conditions
4	i	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	no extra conditions
4	h	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},x,0$	no extra conditions
2	g	2 m m .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			$hk0$: $h+k=2n$
2	f	2 m m .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	e	2 m m .	$0,0,z$	$0,0,\bar{z}$			no extra conditions
1	d	$\bar{4}$ m 2	$0,0,\frac{1}{2}$				no extra conditions
1	c	$\bar{4}$ m 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	b	$\bar{4}$ m 2	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	a	$\bar{4}$ m 2	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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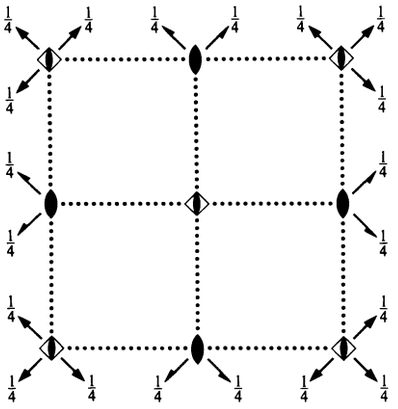
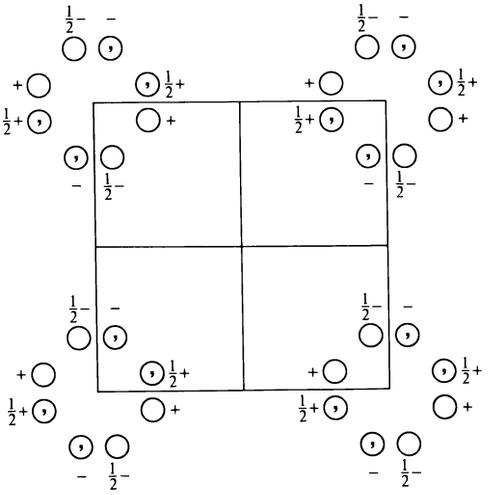
$P\bar{4}c2$ D_{2d}^{6} $\bar{4}m2$ Tetragonal

No. 116 $P\bar{4}c2$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}c1$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^{+}$ $0,0,z$; $0,0,0$ (4) $\bar{4}^{-}$ $0,0,z$; $0,0,0$
(5) c $x,0,z$ (6) c $0,y,z$ (7) 2 $x,x,\frac{1}{4}$ (8) 2 $x,\bar{x},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	$0kl$: $l=2n$
			(5) $x,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},y,z+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
							Special: as above, plus
4	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$ $hk0$: $h+k=2n$
4	h	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	g	2 . .	$0,0,z$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	f	. . 2	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	no extra conditions
4	e	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
2	d	$\bar{4}$ . .	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	c	$\bar{4}$ . .	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
2	b	2 . 22	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	a	2 . 22	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

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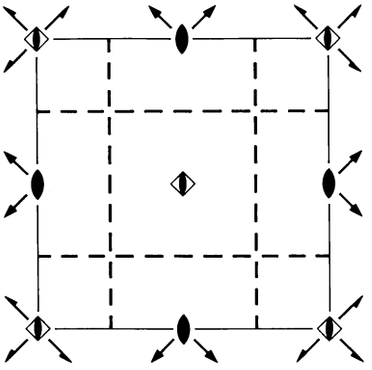
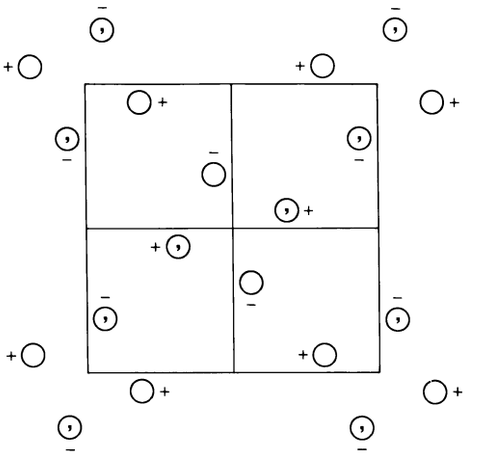
Tetragonal $\bar{4}m2$ D_{2d}^{7} $P\bar{4}b2$

Patterson symmetry $P4/mmm$ $P\bar{4}b2$ No. 117





Origin at $\bar{4}\,1\,2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	$0kl$: $k=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
							Special: as above, plus
4	h	. . 2	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	no extra conditions
4	g	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$	no extra conditions
4	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	hkl: $h+k=2n$
4	e	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hkl: $h+k=2n$
2	d	2 . 2 2	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
2	c	2 . 2 2	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

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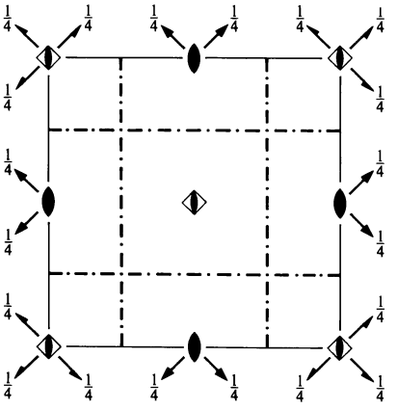
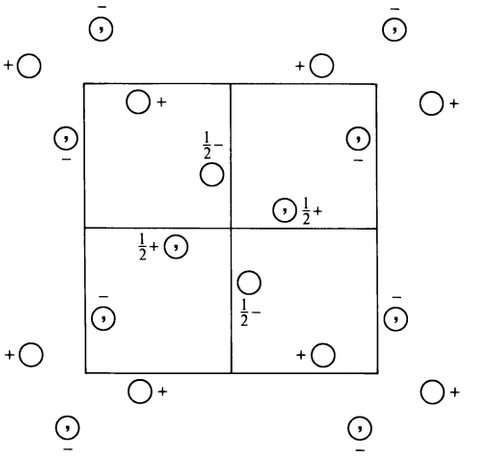
$P\bar{4}n2$ D_{2d}^{8} $\bar{4}m2$ Tetragonal

No. 118 $P\bar{4}n2$ Patterson symmetry $P4/mmm$





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^{+}$ $0,0,z$; $0,0,0$ (4) $\bar{4}^{-}$ $0,0,z$; $0,0,0$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$ (6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$ (7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$ (8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	$0kl$: $k+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	
							Special: as above, plus
4	h	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
4	g	. . 2	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	no extra conditions
4	f	. . 2	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	no extra conditions
4	e	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
2	d	2 . 2 2	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl: $h+k+l=2n$
2	c	2 . 2 2	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$			hkl: $h+k+l=2n$
2	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

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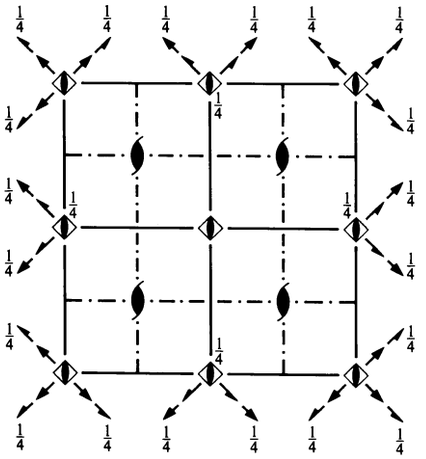
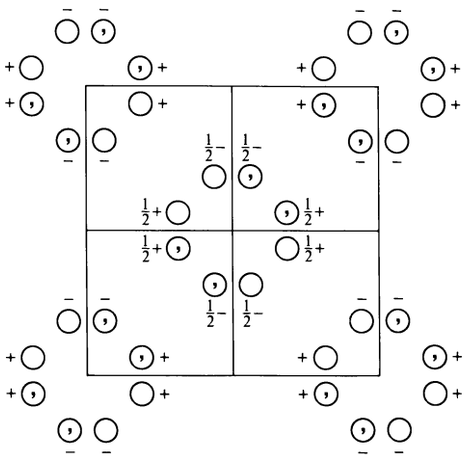
Tetragonal $\bar{4}m2$ D_{2d}^{9} $I\bar{4}m2$

Patterson symmetry $I4/mmm$ $I\bar{4}m2$ No. 119





Origin at $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) m $x,0,z$	(6) m $0,y,z$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(5) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
8	i	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,\bar{x},\bar{z}$	$0,x,\bar{z}$
8	h	$..2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$
8	g	$..2$	$x,x,0$	$\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},x,0$
4	f	$2\,m\,m.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$		
4	e	$2\,m\,m.$	$0,0,z$	$0,0,\bar{z}$		
2	d	$\bar{4}\,m\,2$	$0,\frac{1}{2},\frac{3}{4}$			
2	c	$\bar{4}\,m\,2$	$0,\frac{1}{2},\frac{1}{4}$			
2	b	$\bar{4}\,m\,2$	$0,0,\frac{1}{2}$			
2	a	$\bar{4}\,m\,2$	$0,0,0$			

Reflection conditions

General:

hkl: $h+k+l=2n$
$hk0$: $h+k=2n$
$0kl$: $k+l=2n$
hhl: $l=2n$
$00l$: $l=2n$
$h00$: $h=2n$

Special: no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c1m1$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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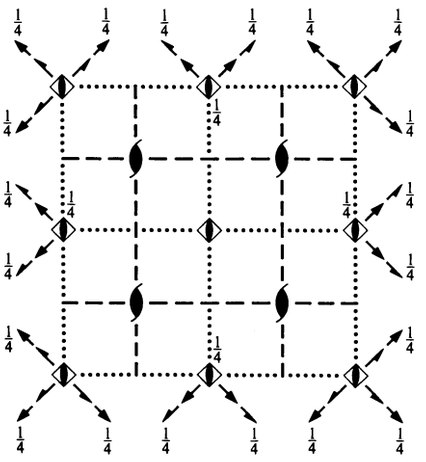
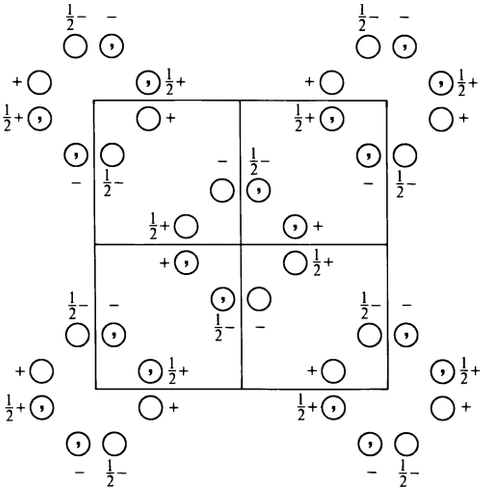
$I\bar{4}c2$ D_{2d}^{10} $\bar{4}m2$ Tetragonal

No. 120 $I\bar{4}c2$ Patterson symmetry $I4/mmm$





Origin at $\bar{4}c2_1$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) c $x,0,z$	(6) c $0,y,z$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(5) a $x,\frac{1}{4},z$	(6) b $\frac{1}{4},y,z$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	i	1	(1) x,y,z (5) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z+\frac{1}{2}$	(3) $y,\bar{x},\bar{z}$ (7) $y,x,\bar{z}+\frac{1}{2}$	(4) $\bar{y},x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k,l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
8	h	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$	no extra conditions
8	g	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
8	f	2 . .	$0,0,z$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
8	e	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
4	d	2 . 22	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $l=2n$
4	c	$\bar{4}$ . .	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	b	$\bar{4}$ . .	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
4	a	2 . 22	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

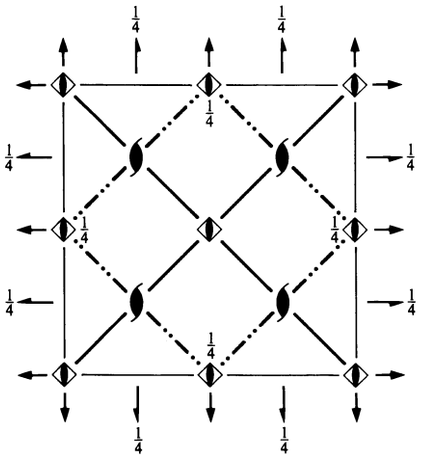
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

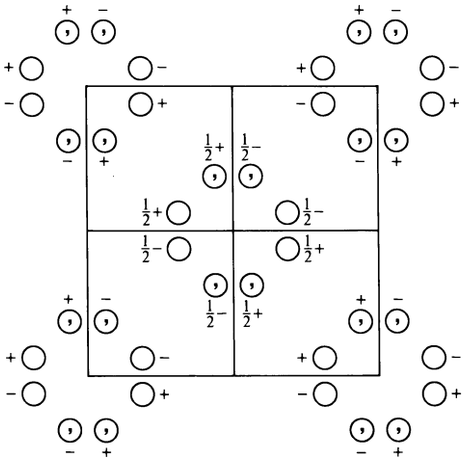
Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$I\bar{4}2m$ D_{2d}^{11} $\bar{4}2m$ Tetragonal

No. 121 $I\bar{4}2m$ Patterson symmetry $I4/mmm$





Origin at $\bar{4}2m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le y$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) $\bar{4}^+$ $0,0,z$; $0,0,0$ (4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) 2 $0,y,0$ (6) 2 $x,0,0$ (7) m $x,\bar{x},z$ (8) m x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (3) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$ (4) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$ (7) c $x+\frac{1}{2},\bar{x},z$ (8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
16	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	hkl: $h+k+l=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $\bar{y},\bar{x},z$	(8) y,x,z	$hk0$: $h+k=2n$
							$0kl$: $k+l=2n$
							hhl: $l=2n$
							$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
8	i	$..m$	x,x,z	$\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$	$\bar{x},x,\bar{z}$	no extra conditions
8	h	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,z$	hkl: $l=2n$
8	g	$.2.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	no extra conditions
8	f	$.2.$	$x,0,0$	$\bar{x},0,0$	$0,\bar{x},0$	$0,x,0$	no extra conditions
4	e	$2.mm$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	$\bar{4}..$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	c	$222.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $l=2n$
2	b	$\bar{4}2m$	$0,0,\frac{1}{2}$				no extra conditions
2	a	$\bar{4}2m$	$0,0,0$				no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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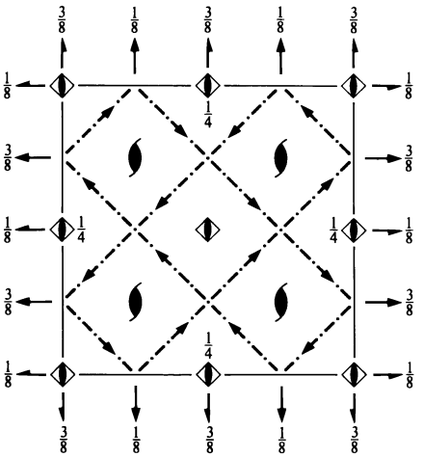
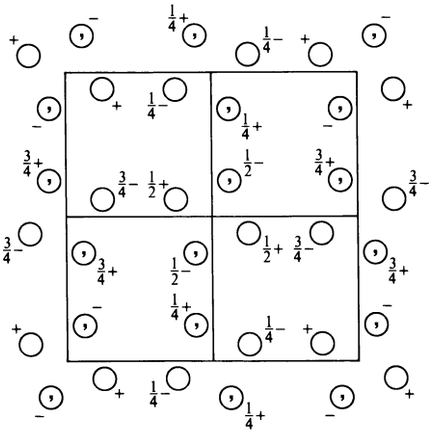
Tetragonal $\bar{4}2m$ D_{2d}^{12} $I\bar{4}2d$

Patterson symmetry $I4/mmm$ $I\bar{4}2d$ No. 122





Origin at $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) $\bar{4}^+$ $0,0,z$; $0,0,0$	(4) $\bar{4}^-$ $0,0,z$; $0,0,0$
(5) 2 $\frac{1}{4},y,\frac{3}{8}$	(6) $2(\frac{1}{2},0,0)$ $x,0,\frac{3}{8}$	(7) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(4) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{8}$	(6) 2 $x,\frac{1}{4},\frac{1}{8}$	(7) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(8) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$		$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$		Reflection conditions
							General:
16	e	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $y,\bar{x},\bar{z}$	(4) $\bar{y},x,\bar{z}$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $2h+l=4n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{3}{4}$	(7) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(8) $y+\frac{1}{2},x,z+\frac{3}{4}$	
							Special: as above, plus
8	d	. 2 .	$x,\frac{1}{4},\frac{1}{8}$	$\bar{x},\frac{3}{4},\frac{1}{8}$	$\frac{1}{4},\bar{x},\frac{7}{8}$	$\frac{3}{4},x,\frac{7}{8}$	no extra conditions
8	c	2 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},0,z+\frac{3}{4}$	hkl: $l=2n+1$ or $2h+l=4n$
4	b	$\bar{4}$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$			hkl: $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},0,\frac{3}{4}$			hkl: $l=2n+1$ or $2h+l=4n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $c1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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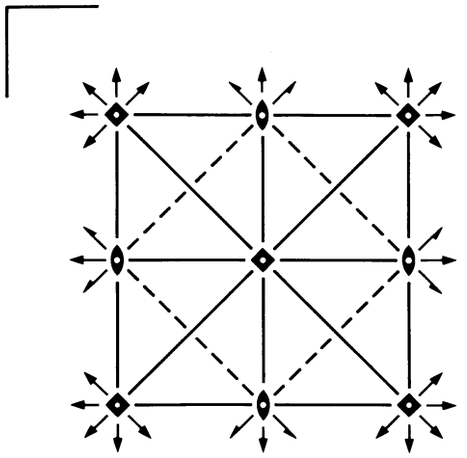
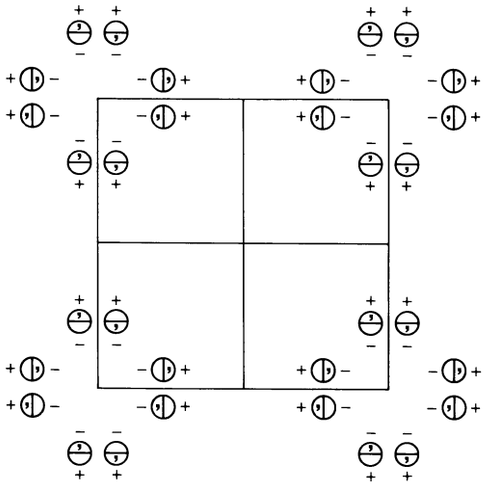
$P4/mmm$ D_{4h}^{1} $4/mmm$ Tetragonal

No. 123 $P\ 4/m\ 2/m\ 2/m$ Patterson symmetry $P4/mmm$





Origin at centre $(4/mmm)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $0,0,0$	(10) m $x,y,0$	(11) $\bar{4}^+$ $0,0,z;\ 0,0,0$	(12) $\bar{4}^-$ $0,0,z;\ 0,0,0$
(13) m $x,0,z$	(14) m $0,y,z$	(15) m $x,\bar{x},z$	(16) m x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	u	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (14) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) y,x,z	no conditions
							Special:
8	t	$.m.$	$x,\frac{1}{2},z$ $\bar{x},\frac{1}{2},\bar{z}$	$\bar{x},\frac{1}{2},z$ $x,\frac{1}{2},\bar{z}$	$\frac{1}{2},x,z$ $\frac{1}{2},x,\bar{z}$	$\frac{1}{2},\bar{x},z$ $\frac{1}{2},\bar{x},\bar{z}$	no extra conditions
8	s	$.m.$	$x,0,z$ $\bar{x},0,\bar{z}$	$\bar{x},0,z$ $x,0,\bar{z}$	$0,x,z$ $0,x,\bar{z}$	$0,\bar{x},z$ $0,\bar{x},\bar{z}$	no extra conditions
8	r	$..m$	x,x,z $\bar{x},x,\bar{z}$	$\bar{x},\bar{x},z$ $x,\bar{x},\bar{z}$	$\bar{x},x,z$ $x,x,\bar{z}$	$x,\bar{x},z$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
8	q	$m..$	$x,y,\frac{1}{2}$ $\bar{x},y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$ $x,\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$ $y,x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$ $\bar{y},\bar{x},\frac{1}{2}$	no extra conditions
8	p	$m..$	$x,y,0$ $\bar{x},y,0$	$\bar{x},\bar{y},0$ $x,\bar{y},0$	$\bar{y},x,0$ $y,x,0$	$y,\bar{x},0$ $\bar{y},\bar{x},0$	no extra conditions
4	o	$m2m.$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	n	$m2m.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	m	$m2m.$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
4	l	$m2m.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	k	$m.2m$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	no extra conditions
4	j	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	i	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $h+k=2n$
2	h	$4mm$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			no extra conditions
2	g	$4mm$	$0,0,z$	$0,0,\bar{z}$			no extra conditions
2	f	$mmm.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
2	e	$mmm.$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
1	d	$4/mmm$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				no extra conditions
1	c	$4/mmm$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
1	b	$4/mmm$	$0,0,\frac{1}{2}$				no extra conditions
1	a	$4/mmm$	$0,0,0$				no extra conditions

Symmetry of special projections

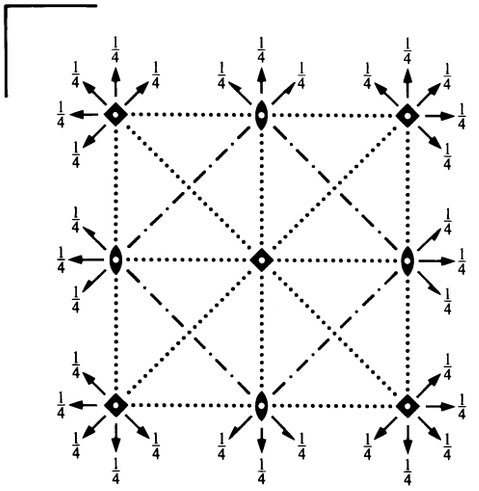
Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

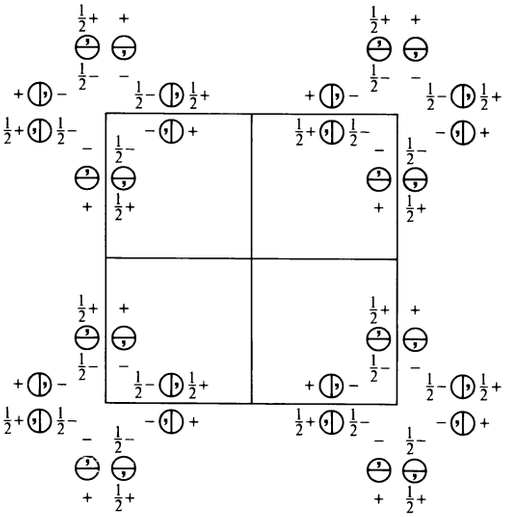
Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$P4/mcc$ D_{4h}^2 $4/mmm$ Tetragonal

No. 124 $P\ 4/m\ 2/c\ 2/c$ Patterson symmetry $P4/mmm$





Origin at centre $(4/m)$ at $4/mcc$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) 4^+ $0,0,z$
(4) 4^- $0,0,z$
(5) 2 $0,y,\frac{1}{4}$
(6) 2 $x,0,\frac{1}{4}$
(7) 2 $x,x,\frac{1}{4}$
(8) 2 $x,\bar{x},\frac{1}{4}$
(9) $\bar{1}$ $0,0,0$
(10) m $x,y,0$
(11) $\bar{4}^+$ $0,0,z;\ 0,0,0$
(12) $\bar{4}^-$ $0,0,z;\ 0,0,0$
(13) c $x,0,z$
(14) c $0,y,z$
(15) c $x,\bar{x},z$
(16) c x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $l=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	hhl: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$	
							Special: as above, plus
8	m	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	
8	l	. 2 .	$x,\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},x,\frac{1}{4}$	$\frac{1}{2},\bar{x},\frac{1}{4}$	hkl: $l=2n$
			$\bar{x},\frac{1}{2},\frac{3}{4}$	$x,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\bar{x},\frac{3}{4}$	$\frac{1}{2},x,\frac{3}{4}$	
8	k	. 2 .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$0,\bar{x},\frac{1}{4}$	hkl: $l=2n$
			$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$	
8	j	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	hkl: $l=2n$
			$\bar{x},\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
8	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	
4	h	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
4	g	4 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
4	f	2 2 2 .	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k,l=2n$
4	e	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h+k,l=2n$
2	d	$4/m$ . .	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	c	4 2 2	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	b	$4/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
2	a	4 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

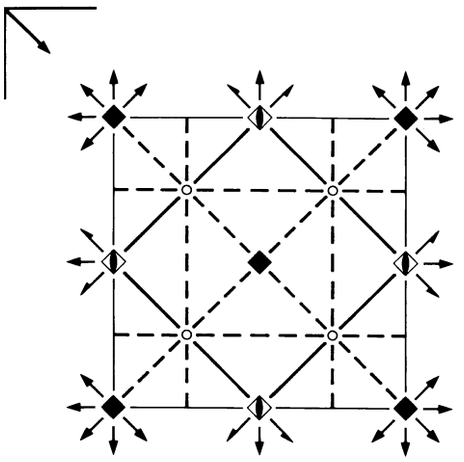
Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

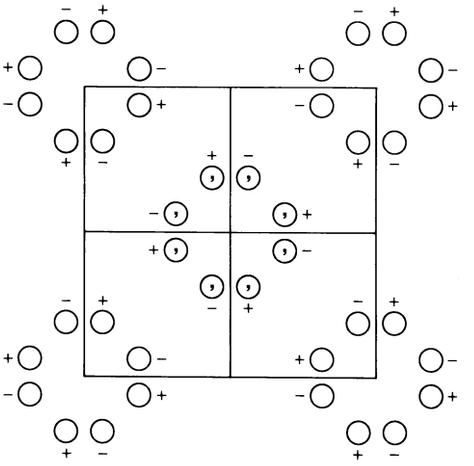
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4/nbm$ D_{4h}^3 $4/mmm$ Tetragonal

No. 125 $P\ 4/n\ 2/b\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at 422 at $4/n22/g$, at $-\frac{1}{4},-\frac{1}{4},0$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) 4^+ $0,0,z$
(4) 4^- $0,0,z$
(5) 2 $0,y,0$
(6) 2 $x,0,0$
(7) 2 $x,x,0$
(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,0$
(12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},0$
(13) a $x,\frac{1}{4},z$
(14) b $\frac{1}{4},y,z$
(15) m $x+\frac{1}{2},\bar{x},z$
(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0kl$: $k=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	m	. . m	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}$	$x,\bar{x}+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},x,\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	
8	l	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	k	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	
8	j	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	i	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	
4	h	2 . mm	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $h+k=2n$
4	g	4 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl: $h+k=2n$
4	f	. . 2/m	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	hkl: $h,k=2n$
4	e	. . 2/m	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	hkl: $h,k=2n$
2	d	$\bar{4}$ 2 m	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
2	c	$\bar{4}$ 2 m	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
2	b	4 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	4 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

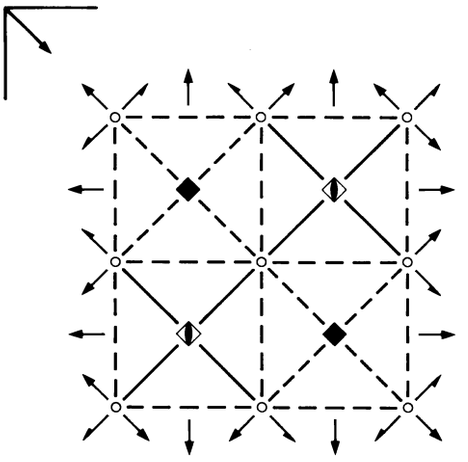
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

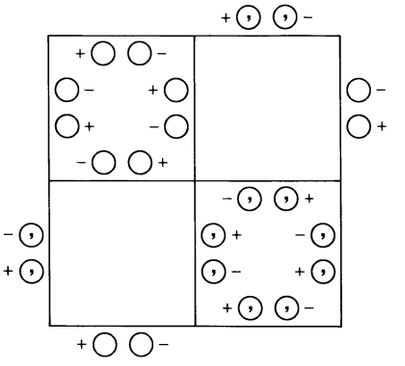
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

No. 125 $P\ 4/n\ 2/b\ 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n(b,a)(2_1/g,2/m)$, at $\frac{1}{4},\frac{1}{4},0$ from 422

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}; \quad x \le -y$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 4^+ $\frac{1}{4},\frac{1}{4},z$	(4) 4^- $\frac{1}{4},\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,0$	(6) 2 $x,\frac{1}{4},0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}$ $0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(11) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z;$ $\frac{1}{4},-\frac{1}{4},0$	(12) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z;$ $-\frac{1}{4},\frac{1}{4},0$
(13) a $x,0,z$	(14) b $0,y,z$	(15) m $x,\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	m	. . m	$x,\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z$	$x+\frac{1}{2},x,z$	$\bar{x},\bar{x}+\frac{1}{2},z$	no extra conditions
			$\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},x,\bar{z}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
8	l	. 2 .	$x,\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},x,\frac{1}{2}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x},\frac{3}{4},\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\bar{x},\frac{1}{2}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{2}$	
8	k	. 2 .	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\frac{1}{4},x,0$	$\frac{1}{4},\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	$\frac{3}{4},\bar{x},0$	$\frac{3}{4},x+\frac{1}{2},0$	
8	j	. . 2	$x,x,\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x},\bar{x},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$	
8	i	. . 2	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x,\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x},\bar{x},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},0$	$\bar{x},x+\frac{1}{2},0$	
4	h	2 . mm	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	hkl: $h+k=2n$
4	g	4 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z$	hkl: $h+k=2n$
4	f	. . $2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h,k=2n$
4	e	. . $2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h,k=2n$
2	d	$\bar{4}$ 2 m	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	c	$\bar{4}$ 2 m	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hkl: $h+k=2n$
2	b	4 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	a	4 2 2	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

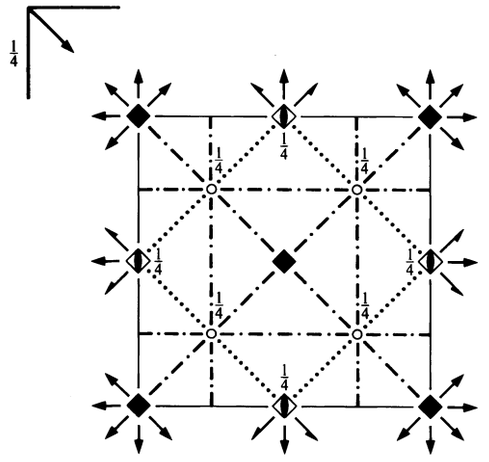
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

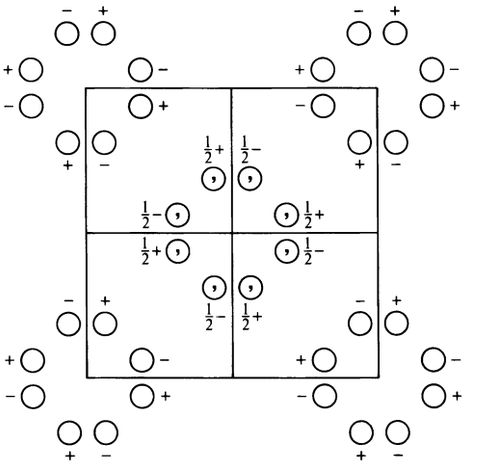
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$P4/nnc$ D_{4h}^4 $4/mmm$ Tetragonal

No. 126 $P\ 4/n\ 2/n\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $42\,2/n$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(15) c $x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0kl$: $k+l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
8	j	. 2 .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	
8	i	. 2 .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	h	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
8	g	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl: $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	
8	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl: $h,k,l=2n$
			$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	
4	e	4 . .	$0,0,z$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	d	$\bar{4}$ . .	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl: $h+k,l=2n$
4	c	2 2 2 .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	hkl: $h+k,l=2n$
2	b	4 2 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	4 2 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

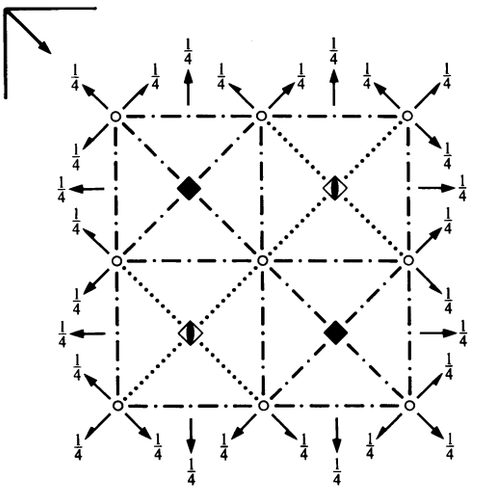
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

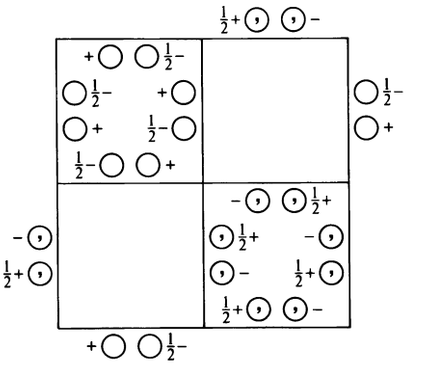
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

No. 126 $P\ 4/n\ 2/n\ 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $nn(n,c)$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 422

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) 4^+ $\frac{1}{4},\frac{1}{4},z$
(4) 4^- $\frac{1}{4},\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,\frac{1}{4}$
(6) 2 $x,\frac{1}{4},\frac{1}{4}$
(7) 2 $x,x,\frac{1}{4}$
(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}$ $0,0,0$
(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(11) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z; \quad \frac{1}{4},-\frac{1}{4},0$
(12) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z; \quad -\frac{1}{4},\frac{1}{4},0$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$
(14) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
(15) c $x,\bar{x},z$
(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
16	k	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$					$hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$					
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$					
			(13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$					
											Special: as above, plus
8	j	. 2 .	$x,\frac{3}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$					hkl: $h+k+l=2n$
			$\bar{x},\frac{1}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x+\frac{1}{2},\frac{3}{4}$					
8	i	. 2 .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$					hkl: $h+k+l=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$					
8	h	. . 2	$x,x,\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$					hkl: $h+k+l=2n$
			$\bar{x},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x},x+\frac{1}{2},\frac{3}{4}$					
8	g	2 . .	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$					hkl: $h+k,l=2n$
			$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$					
8	f	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h,k,l=2n$
4	e	4 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$					hkl: $h+k+l=2n$
4	d	$\bar{4}$ . .	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$					hkl: $h+k,l=2n$
4	c	2 2 2 .	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$					hkl: $h+k,l=2n$
2	b	4 2 2	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$							hkl: $h+k+l=2n$
2	a	4 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$							hkl: $h+k+l=2n$

Symmetry of special projections

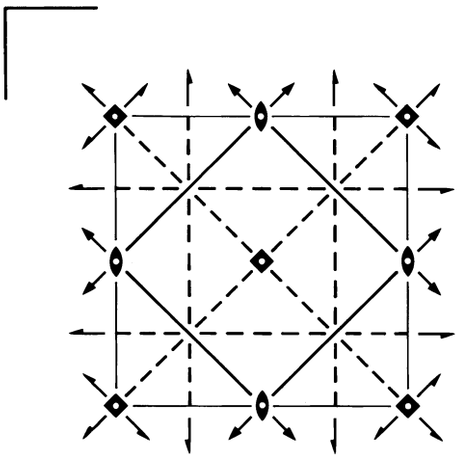
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

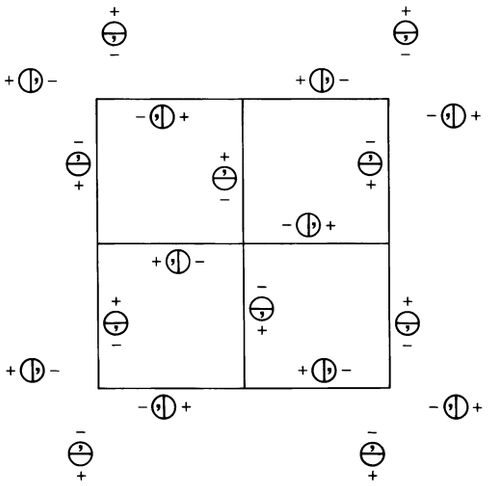
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4/mbm$ D_{4h}^5 $4/mmm$ Tetragonal

No. 127 $P\ 4/m\ 2_1/b\ 2/m$ Patterson symmetry $P4/mmm$





Origin at centre $(4/m)$ at $4/m1 2_1/g$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}$ $0,0,0$	(10) m $x,y,0$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) a $x,\frac{1}{4},z$	(14) b $\frac{1}{4},y,z$	(15) m $x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	k	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x,x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x}+\frac{1}{2},\bar{z}$	
8	j	$m..$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	
4	h	$m.2m$	$x,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	g	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
4	f	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	hkl: $h+k=2n$
4	e	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	hkl: $h+k=2n$
2	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k=2n$
2	c	$m.mm$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k=2n$
2	b	$4/m..$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$4/m..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

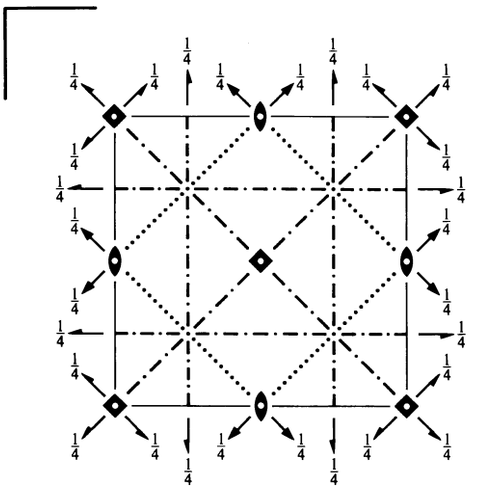
Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

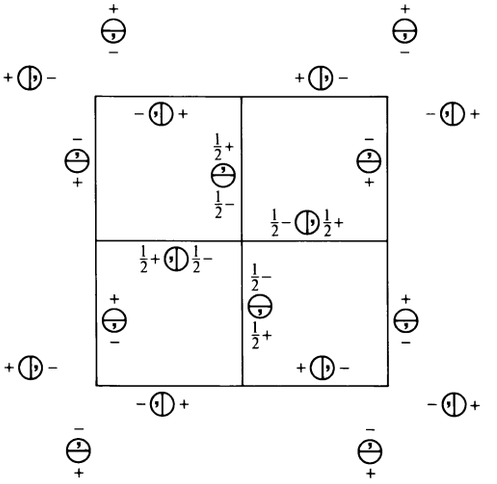
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$P4/mnc$ D_{4h}^6 $4/mmm$ Tetragonal

No. 128 $P\ 4/m\ 2_1/n\ 2/c$ Patterson symmetry $P4/mmm$





Origin at centre $(4/m)$ at $4/m\,1\,n$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) 4^+ $0,0,z$
(4) 4^- $0,0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$
(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$
(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}$ $0,0,0$
(10) m $x,y,0$
(11) $\bar{4}^+$ $0,0,z$; $0,0,0$
(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$
(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(15) c $x+\frac{1}{2},\bar{x},z$
(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k+l=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
8	h	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	g	. . 2	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	hkl: $l=2n$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	
8	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	
4	e	4 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	hkl: $h+k+l=2n$
4	d	2 . 2 2	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k,l=2n$
4	c	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h+k,l=2n$
2	b	$4/m$ . .	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$4/m$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

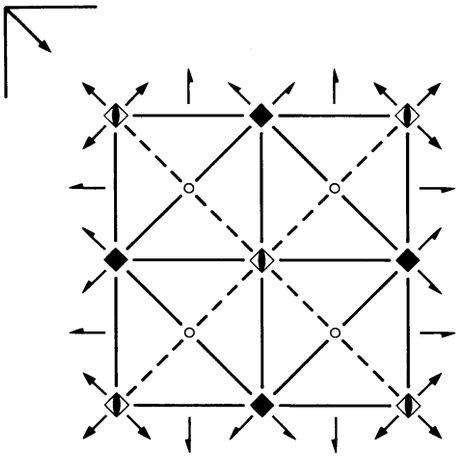
Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

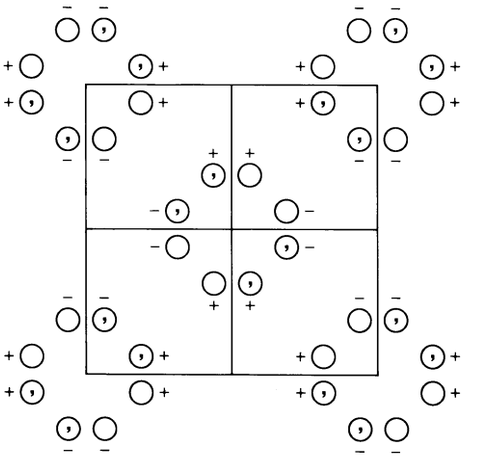
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4/nmm$ D_{4h}^{7} $4/mmm$ Tetragonal

No. 129 $P\ 4/n\ 2_1/m\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2$ at $\bar{4}/nm2/g$, at $-\frac{1}{4},\frac{1}{4},0$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) 4^+ $0,\frac{1}{2},z$
(4) 4^- $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(7) 2 $x,x,0$
(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(11) $\bar{4}^+$ $0,0,z;\ 0,0,0$
(12) $\bar{4}^-$ $0,0,z;\ 0,0,0$
(13) m $x,0,z$
(14) m $0,y,z$
(15) m $x+\frac{1}{2},\bar{x},z$
(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	
							Special: as above, plus
8	j	. . m	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x},x+\frac{1}{2},z$	$x,\bar{x}+\frac{1}{2},z$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x+\frac{1}{2},x,\bar{z}$	$\bar{x}+\frac{1}{2},\bar{x},\bar{z}$	
8	i	. m .	$0,y,z$	$0,\bar{y},z$	$\bar{y}+\frac{1}{2},\frac{1}{2},z$	$y+\frac{1}{2},\frac{1}{2},z$	no extra conditions
			$\frac{1}{2},y+\frac{1}{2},\bar{z}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	
8	h	. . 2	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	
8	g	. . 2	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x,\bar{x},0$	$\bar{x},x,0$	
4	f	2 m m .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	hkl: $h+k=2n$
4	e	. . $2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl: $h,k=2n$
4	d	. . $2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h,k=2n$
2	c	4 m m	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$			no extra conditions
2	b	$\bar{4}$ m 2	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}$ m 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

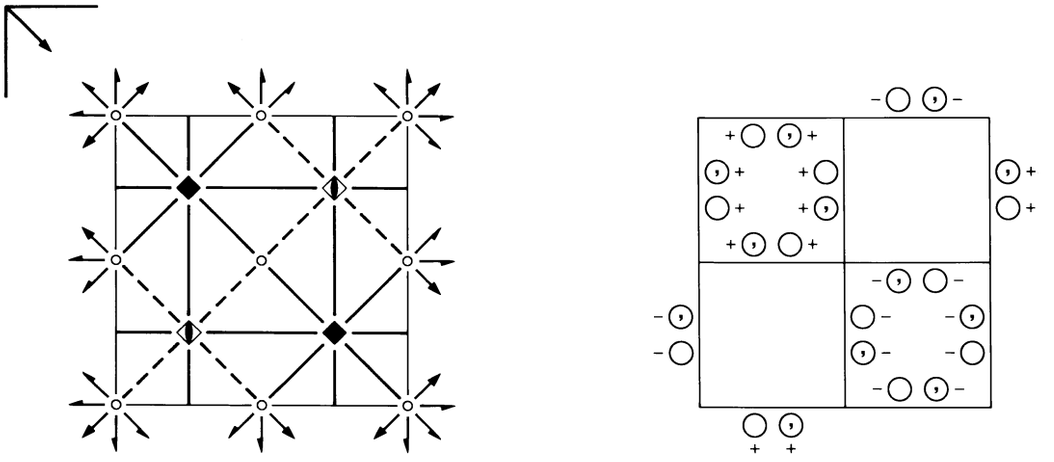
Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

No. 129 $P\ 4/n\ 2_1/m\ 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2



Origin at centre $(2/m)$ at $n2_1(2/m,2_1/g)$, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}m2$

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{4};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{2};\quad x\le y$

Symmetry operations

(1) 1
(2) $2\ \frac{1}{4},\frac{1}{4},z$
(3) $4^+\ \frac{1}{4},\frac{1}{4},z$
(4) $4^-\ \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,0$
(6) $2(\frac{1}{2},0,0)\ \ x,0,0$
(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,0$
(8) $2\ \ x,\bar{x},0$
(9) $\bar{1}\ \ 0,0,0$
(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$
(11) $\bar{4}^+\ \frac{1}{4},-\frac{1}{4},z;\ \ \frac{1}{4},-\frac{1}{4},0$
(12) $\bar{4}^-\ -\frac{1}{4},\frac{1}{4},z;\ \ -\frac{1}{4},\frac{1}{4},0$
(13) $m\ \ x,\frac{1}{4},z$
(14) $m\ \ \frac{1}{4},y,z$
(15) $m\ \ x+\frac{1}{2},\bar{x},z$
(16) $m\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$h00$: $h=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$	
			(13) $x,\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) y,x,z	
							Special: as above, plus
8	j	$..m$	x,x,z	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x,\bar{x}+\frac{1}{2},z$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	i	$.m.$	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$	$\bar{y}+\frac{1}{2},\frac{1}{4},z$	$y,\frac{1}{4},z$	no extra conditions
			$\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	$y+\frac{1}{2},\frac{3}{4},\bar{z}$	$\bar{y},\frac{3}{4},\bar{z}$	
8	h	$..2$	$x,\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x,\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x},\frac{1}{2}$	$x,x+\frac{1}{2},\frac{1}{2}$	
8	g	$..2$	$x,\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},x,0$	$\bar{x},\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x},x,0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\bar{x},0$	$x,x+\frac{1}{2},0$	
4	f	$2\,m\,m.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	hkl: $h+k=2n$
4	e	$..2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h,k=2n$
4	d	$..2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h,k=2n$
2	c	$4\,m\,m$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}$			no extra conditions
2	b	$\bar{4}\,m\,2$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$			hkl: $h+k=2n$
2	a	$\bar{4}\,m\,2$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$			hkl: $h+k=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

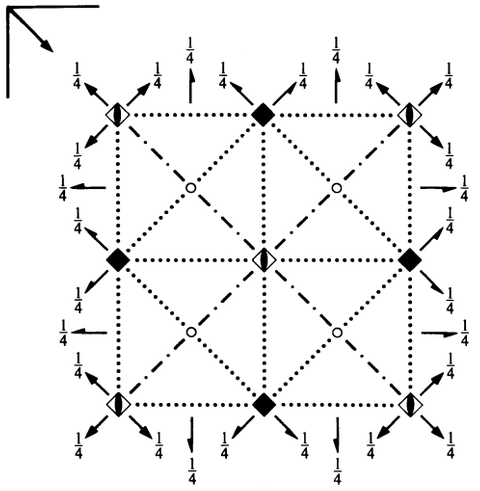
Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

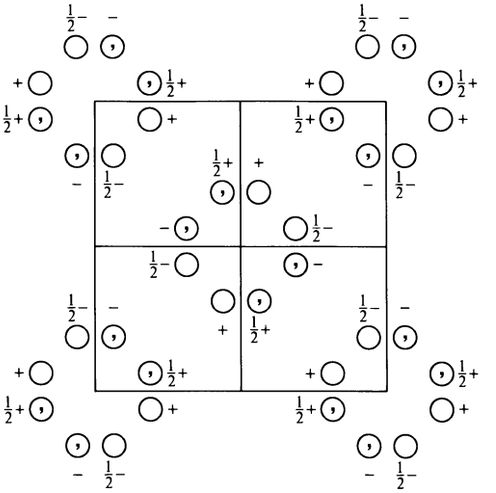
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$P4/ncc$ D_{4h}^{8} $4/mmm$ Tetragonal

No. 130 $P\ 4/n\ 2_1/c\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}/ncn$, at $-\frac{1}{4},\frac{1}{4},0$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,\frac{1}{2},z$	(4) 4^- $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},\frac{1}{4}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) c $x,0,z$	(14) c $0,y,z$	(15) c $x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	g	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$0kl$: $l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	hhl: $l=2n$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$00l$: $l=2n$
							$h00$: $h=2n$
							Special: as above, plus
8	f	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
8	e	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	hkl: $h+k,l=2n$
			$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	
8	d	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$ $\frac{3}{4},\frac{1}{4},\frac{1}{2}$ $\frac{1}{4},\frac{1}{4},\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},\frac{1}{2}$ hkl: $h,k,l=2n$
4	c	4 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
4	b	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	hkl: $h+k,l=2n$
4	a	2 . 22	$0,0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$0,0,\frac{3}{4}$	hkl: $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{4},0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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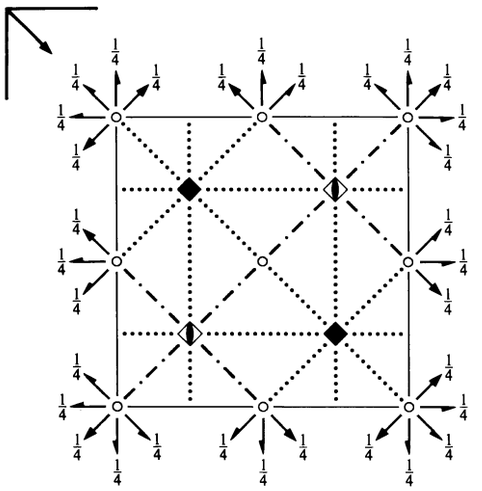
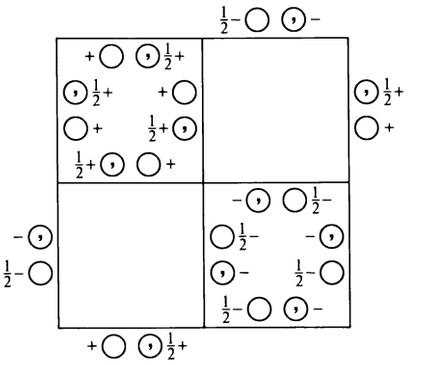
Patterson symmetry $P4/mmm$

$P\ 4/n\ 2_1/c\ 2/c$ No. 130

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $n1\,(c,n)$, at $\frac{1}{4},-\frac{1}{4},0$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{4};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \frac{1}{4},\frac{1}{4},z$	(3) $4^+\ \frac{1}{4},\frac{1}{4},z$	(4) $4^-\ \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(11) $\bar{4}^+\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},0$	(12) $\bar{4}^-\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},0$
(13) $c\ \ x,\frac{1}{4},z$	(14) $c\ \ \frac{1}{4},y,z$	(15) $c\ \ x+\frac{1}{2},\bar{x},z$	(16) $c\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
16	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z$	(4) $y,\bar{x}+\frac{1}{2},z$					$hk0$: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$					$0kl$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}$					hhl: $l=2n$
			(13) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$					$00l$: $l=2n$
											$h00$: $h=2n$
											Special: as above, plus
8	f	$..2$	$x,\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x,\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$					hkl: $h+k+l=2n$
			$\bar{x},x,\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\bar{x},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$					
8	e	$2..$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$					hkl: $h+k,l=2n$
			$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$					
8	d	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	hkl: $h,k,l=2n$
4	c	$4..$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$					hkl: $l=2n$
4	b	$\bar{4}..$	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$					hkl: $h+k,l=2n$
4	a	2.22	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$					hkl: $h+k,l=2n$

Symmetry of special projections

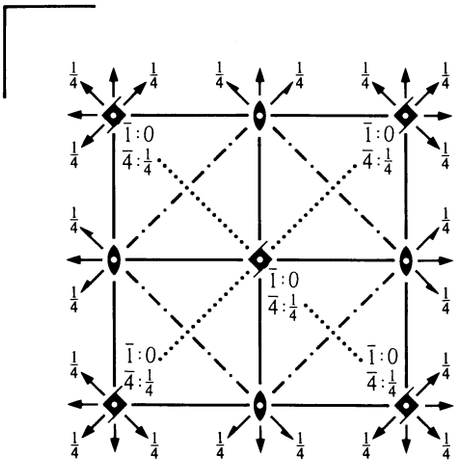
Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

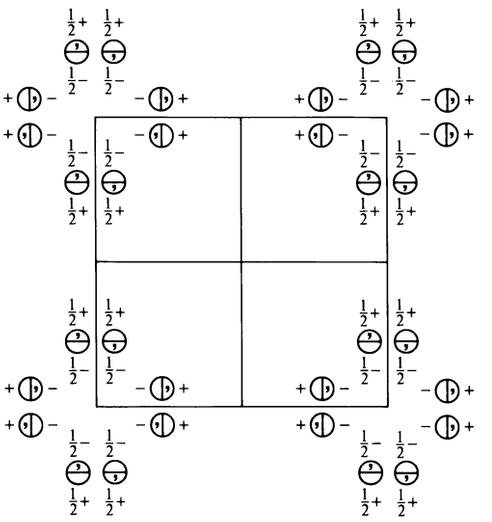
Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4_2/mmc$ D_{4h}^9 $4/mmm$ Tetragonal

No. 131 $P\ 4_2/m\ 2/m\ 2/c$ Patterson symmetry $P4/mmm$





Origin at centre (mmm) at $4_2/m2/mc$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{1}{2})$ $0,0,z$	(4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},\frac{1}{4}$
(9) $\bar{1}$ $0,0,0$	(10) m $x,y,0$	(11) $\bar{4}^+$ $0,0,z;$ $0,0,\frac{1}{4}$	(12) $\bar{4}^-$ $0,0,z;$ $0,0,\frac{1}{4}$
(13) m $x,0,z$	(14) m $0,y,z$	(15) c $x,\bar{x},z$	(16) c x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	r	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	hhl: $l=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$	
							Special: as above, plus
8	q	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x},y,0$	$x,\bar{y},0$	$y,x,\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$	
8	p	. m .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\bar{y},\frac{1}{2},z+\frac{1}{2}$	$y,\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$y,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{y},\frac{1}{2},\bar{z}+\frac{1}{2}$	
8	o	. m .	$0,y,z$	$0,\bar{y},z$	$\bar{y},0,z+\frac{1}{2}$	$y,0,z+\frac{1}{2}$	no extra conditions
			$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$y,0,\bar{z}+\frac{1}{2}$	$\bar{y},0,\bar{z}+\frac{1}{2}$	
8	n	. . 2	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{3}{4}$	$x,\bar{x},\frac{3}{4}$	hkl: $l=2n$
			$\bar{x},\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	
4	m	m 2 m.	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	no extra conditions
4	l	m 2 m.	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,x,0$	$0,\bar{x},0$	no extra conditions
4	k	m 2 m.	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
4	j	m 2 m.	$x,0,0$	$\bar{x},0,0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	no extra conditions
4	i	2 m m.	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
4	h	2 m m.	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	g	2 m m.	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
2	f	$\bar{4}$ m 2	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	e	$\bar{4}$ m 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$
2	d	m m m.	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$			hkl: $h+k+l=2n$
2	c	m m m.	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$			hkl: $h+k+l=2n$
2	b	m m m.	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	a	m m m.	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

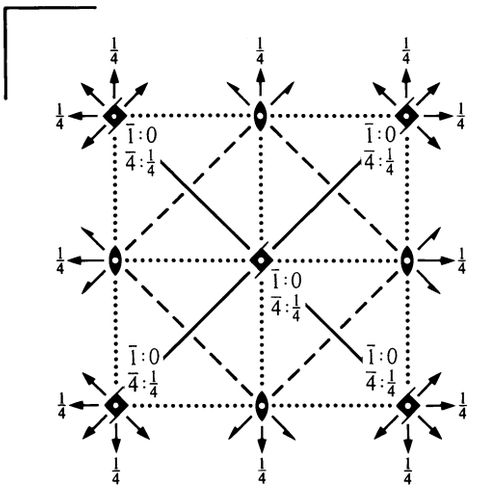
Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

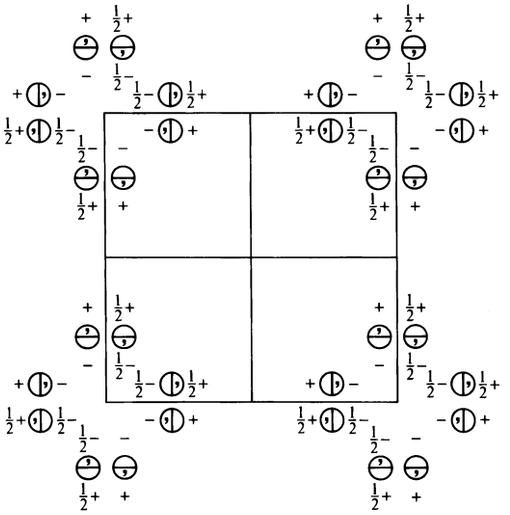
Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4_2/mcm$ D_{4h}^{10} $4/mmm$ Tetragonal

No. 132 $P\ 4_2/m\ 2/c\ 2/m$ Patterson symmetry $P4/mmm$





Origin at centre (mmm) at $4_2/mc2/m$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) $4^+(0,0,\frac{1}{2})$ $0,0,z$
(4) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(5) 2 $0,y,\frac{1}{4}$
(6) 2 $x,0,\frac{1}{4}$
(7) 2 $x,x,0$
(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $0,0,0$
(10) m $x,y,0$
(11) $\bar{4}^+$ $0,0,z;$ $0,0,\frac{1}{4}$
(12) $\bar{4}^-$ $0,0,z;$ $0,0,\frac{1}{4}$
(13) c $x,0,z$
(14) c $0,y,z$
(15) m $x,\bar{x},z$
(16) m x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	p	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$0kl$: $l=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$00l$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: as above, plus
8	o	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$x,\bar{x},z+\frac{1}{2}$	no extra conditions
			$\bar{x},x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	n	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	$y,x,0$	$\bar{y},\bar{x},0$	
8	m	$.2.$	$x,\frac{1}{2},\frac{1}{4}$	$\bar{x},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},x,\frac{3}{4}$	$\frac{1}{2},\bar{x},\frac{3}{4}$	hkl: $l=2n$
			$\bar{x},\frac{1}{2},\frac{3}{4}$	$x,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\bar{x},\frac{1}{4}$	$\frac{1}{2},x,\frac{1}{4}$	
8	l	$.2.$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$0,x,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	hkl: $l=2n$
			$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$	$0,x,\frac{1}{4}$	
8	k	$2..$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl: $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z$	
4	j	$m.2m$	$x,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
4	i	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	no extra conditions
4	h	$2.mm$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hkl: $l=2n$
4	g	$2.mm$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl: $l=2n$
4	f	$2/m..$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	hkl: $h+k,l=2n$
4	e	$222.$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	hkl: $h+k,l=2n$
2	d	$\bar{4}2m$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
2	c	$m.mm$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
2	b	$\bar{4}2m$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$
2	a	$m.mm$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

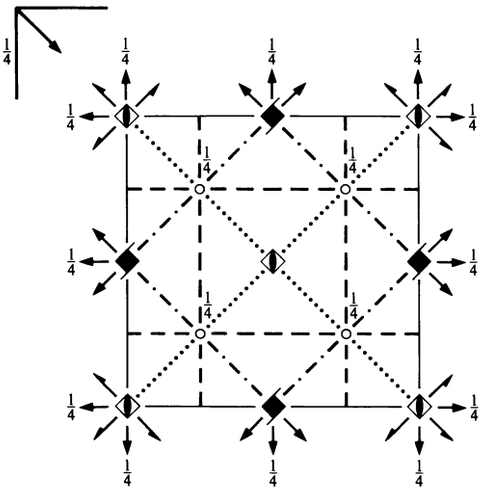
Along [100] $p2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

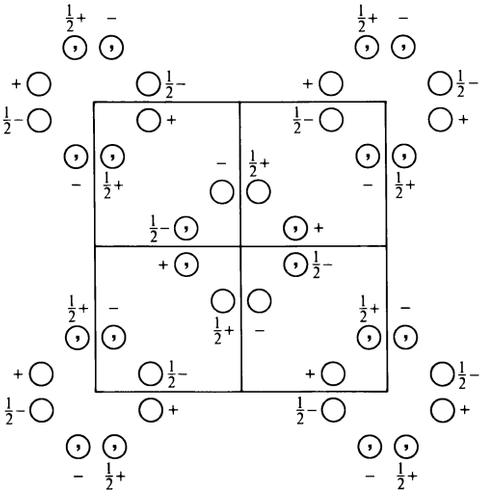
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$P4_2/nbc$ D_{4h}^{11} $4/mmm$ Tetragonal

No. 133 $P\ 4_2/n\ 2/b\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}\,1\,2_1/c$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) 2 $0,y,\frac{1}{4}$	(6) 2 $x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) a $x,\frac{1}{4},z$	(14) b $\frac{1}{4},y,z$	(15) c $x,\bar{x},z$	(16) c x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$					$hk0$: $h+k=2n$
			(5) $\bar{x},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$					$0kl$: $k=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$					hhl: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$					$00l$: $l=2n$
											$h00$: $h=2n$
											Special: as above, plus
8	j	. . 2	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\frac{1}{2}$					hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\bar{x},\frac{1}{2}$	$x+\frac{1}{2},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x},0$	$\bar{x}+\frac{1}{2},x,0$					
8	i	. 2 .	$x,0,\frac{3}{4}$	$\bar{x},0,\frac{3}{4}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$					hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$	$0,x,\frac{1}{4}$					
8	h	. 2 .	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$					hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$0,\bar{x},\frac{3}{4}$	$0,x,\frac{3}{4}$					
8	g	2 . .	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$					hkl: $h+k,l=2n$
			$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$0,0,z+\frac{1}{2}$					
8	f	2 . .	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$					hkl: $h+k,l=2n$
			$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,z$	$\frac{1}{2},0,z+\frac{1}{2}$					
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h,k,l=2n$
4	d	$\bar{4}$ . .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$					hkl: $h+k,l=2n$
4	c	2 . 2 2	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$					hkl: $h+k,l=2n$
4	b	2 2 2 .	$0,0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$0,0,\frac{3}{4}$					hkl: $h+k,l=2n$
4	a	2 2 2 .	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$					hkl: $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

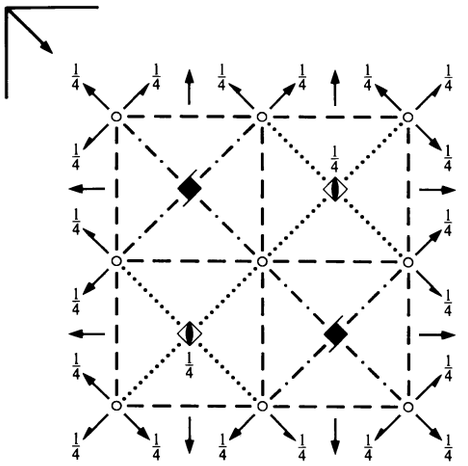
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{4}$

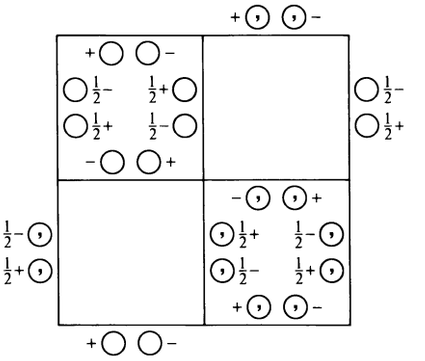
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

No. 133 $P\ 4_2/n\ 2/b\ 2/c$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $n(b,a)(n,c)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,0$	(6) 2 $x,\frac{1}{4},0$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}$ $0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(11) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z;$ $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(12) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z;$ $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(13) a $x,0,z$	(14) b $0,y,z$	(15) c $x,\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
16	k	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$					$hk0$: $h+k=2n$ $0kl$: $k=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$					
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$					
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y+\frac{1}{2},z$	(15) $\bar{y},\bar{x},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$					
											Special: as above, plus
8	j	. . 2	$x,x,\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	$x,\bar{x}+\frac{1}{2},\frac{3}{4}$					hkl: $h+k+l=2n$
			$\bar{x},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$					
8	i	. 2 .	$x,\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},x,0$	$\frac{1}{4},\bar{x}+\frac{1}{2},0$					hkl: $h+k=2n$
			$\bar{x},\frac{3}{4},\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\bar{x},0$	$\frac{3}{4},x+\frac{1}{2},0$					
8	h	. 2 .	$x,\frac{1}{4},0$	$\bar{x}+\frac{1}{2},\frac{1}{4},0$	$\frac{1}{4},x,\frac{1}{2}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{2}$					hkl: $h+k=2n$
			$\bar{x},\frac{3}{4},0$	$x+\frac{1}{2},\frac{3}{4},0$	$\frac{3}{4},\bar{x},\frac{1}{2}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{2}$					
8	g	2 . .	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$					hkl: $h+k,l=2n$
			$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$					
8	f	2 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\bar{z}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$					hkl: $h+k,l=2n$
			$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},z$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$					
8	e	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h,k,l=2n$
4	d	$\bar{4}$ . .	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$					hkl: $h+k,l=2n$
4	c	2 . 2 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$					hkl: $h+k,l=2n$
4	b	2 2 2 .	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$					hkl: $h+k,l=2n$
4	a	2 2 2 .	$\frac{1}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$					hkl: $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

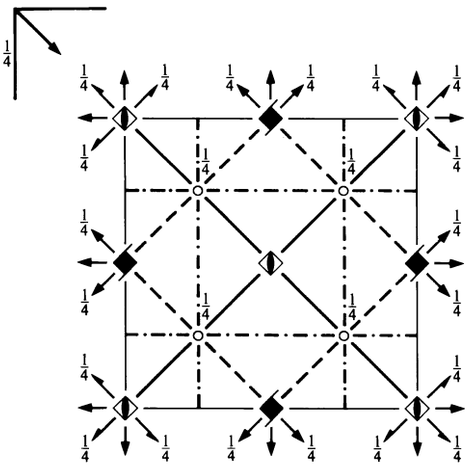
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

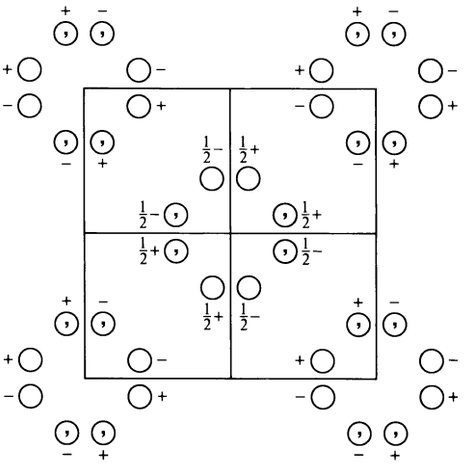
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4_2/nnm$ D_{4h}^{12} $4/mmm$ Tetragonal

No. 134 $P\ 4_2/n\ 2/n\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}\,2m$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le 1$; $0 \le z \le \frac{1}{4}$; $x \le y$; $y \le 1-x$

Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$
(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) 2 $0,y,0$
(6) 2 $x,0,0$
(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$
(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$
(11) $\bar{4}^+$ $0,0,z$; $0,0,0$
(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$
(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(15) m $x,\bar{x},z$
(16) m x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x},y,\bar{z}$	(6) $x,\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	$h00$: $h=2n$
							Special: as above, plus
8	m	. . m	x,x,z $\bar{x},x,\bar{z}$	$\bar{x},\bar{x},z$ $x,\bar{x},\bar{z}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	no extra conditions
8	l	. . 2	$x,x+\frac{1}{2},\frac{3}{4}$ $\bar{x}+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$ $x+\frac{1}{2},x,\frac{3}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$ $x+\frac{1}{2},\bar{x},\frac{1}{4}$	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$ $\bar{x}+\frac{1}{2},x,\frac{1}{4}$	hkl: $h+k=2n$
8	k	. . 2	$x,x+\frac{1}{2},\frac{1}{4}$ $\bar{x}+\frac{1}{2},\bar{x},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$ $x+\frac{1}{2},x,\frac{1}{4}$	$\bar{x},x+\frac{1}{2},\frac{3}{4}$ $x+\frac{1}{2},\bar{x},\frac{3}{4}$	$x,\bar{x}+\frac{1}{2},\frac{3}{4}$ $\bar{x}+\frac{1}{2},x,\frac{3}{4}$	hkl: $h+k=2n$
8	j	. 2 .	$x,0,\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\bar{x},0,\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$ $0,\bar{x},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$ $0,x,\frac{1}{2}$	hkl: $h+k+l=2n$
8	i	. 2 .	$x,0,0$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $0,\bar{x},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $0,x,0$	hkl: $h+k+l=2n$
8	h	2 . .	$0,\frac{1}{2},z$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$ $\frac{1}{2},0,z+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,z$	hkl: $h+k,l=2n$
4	g	2 . mm	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $h+k+l=2n$
4	f	. . $2/m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$
4	e	. . $2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
4	d	2 . 2 2	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k,l=2n$
4	c	2 2 2 .	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	hkl: $h+k,l=2n$
2	b	$\bar{4}$ 2 m	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$\bar{4}$ 2 m	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

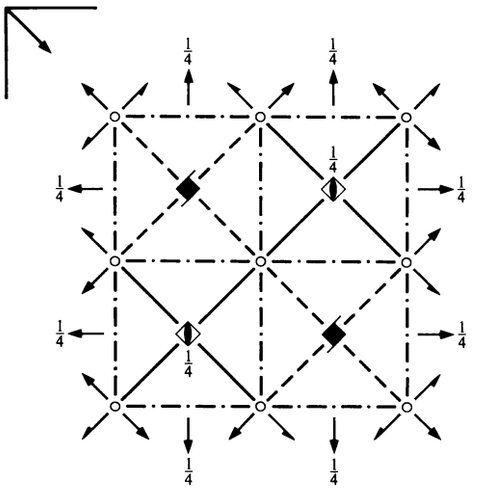
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

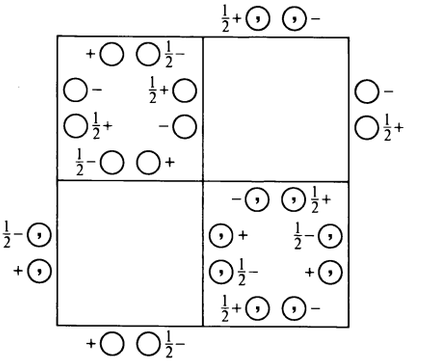
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

No. 134 $P\ 4_2/n\ 2/n\ 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $nn(2_1/g,2/m)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}2m$

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{4};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{2};\quad x\le -y$

Symmetry operations

(1) 1
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) $4^+(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,\frac{1}{4}$
(6) 2 $x,\frac{1}{4},\frac{1}{4}$
(7) 2 $x,x,0$
(8) 2 $x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}$ $0,0,0$
(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(11) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(12) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$
(14) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
(15) m $x,\bar{x},z$
(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	n	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	$0kl$: $k+l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
			(13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	$h00$: $h=2n$
							Special: as above, plus
8	m	. . m	$x,\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z$	$x+\frac{1}{2},x,z+\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	$x,x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{x},x,\bar{z}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
8	l	. . 2	$x,x,\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,0$	$x,\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x},\bar{x},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},0$	$\bar{x},x+\frac{1}{2},0$	
8	k	. . 2	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x},\bar{x},0$	$x+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},\bar{x},\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$	
8	j	. 2 .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	hkl: $h+k+l=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{1}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	
8	i	. 2 .	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	hkl: $h+k+l=2n$
			$\bar{x},\frac{3}{4},\frac{1}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	
8	h	2 . .	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\bar{z}$	hkl: $h+k,l=2n$
			$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},z$	
4	g	2 . mm	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	hkl: $h+k+l=2n$
4	f	. . $2/m$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
4	e	. . $2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h+k,h+l,k+l=2n$
4	d	2 . 2 2	$\frac{1}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$	hkl: $h+k,l=2n$
4	c	2 2 2 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	hkl: $h+k,l=2n$
2	b	$\bar{4}$ 2 m	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k+l=2n$
2	a	$\bar{4}$ 2 m	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			hkl: $h+k+l=2n$

Symmetry of special projections

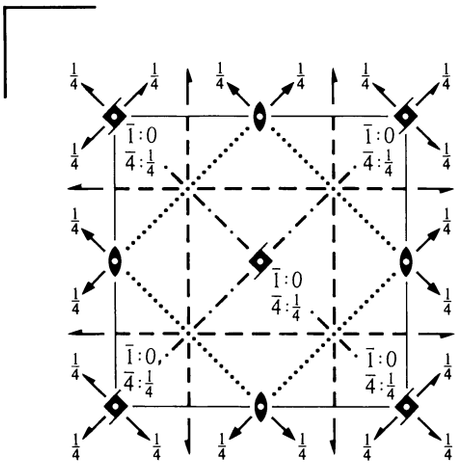
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

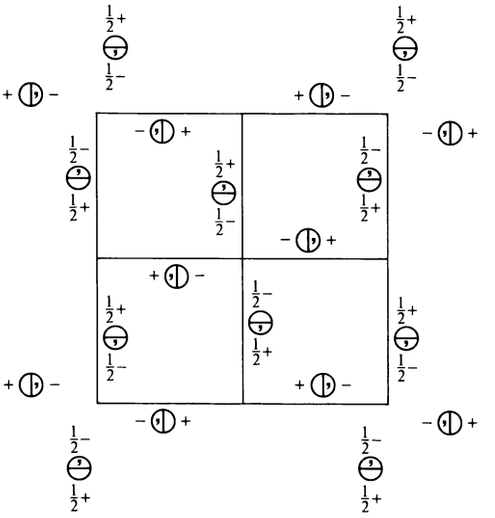
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$P4_2/mbc$ D_{4h}^{13} $4/mmm$ Tetragonal

No. 135 $P\ 4_2/m\ 2_1/b\ 2/c$ Patterson symmetry $P4/mmm$





Origin at centre $(2/m)$ at $4_2/m\,1\,n$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\ 0,0,z$	(4) $4^-(0,0,\frac{1}{2})\ 0,0,z$
(5) $2(0,\frac{1}{2},0)\ \frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)\ x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ x,x,\frac{1}{4}$	(8) $2\ x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}\ 0,0,0$	(10) $m\ x,y,0$	(11) $\bar{4}^+\ 0,0,z;\ 0,0,\frac{1}{4}$	(12) $\bar{4}^-\ 0,0,z;\ 0,0,\frac{1}{4}$
(13) $a\ x,\frac{1}{4},z$	(14) $b\ \frac{1}{4},y,z$	(15) $c\ x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ x,x,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z+\frac{1}{2}$	(4) $y,\bar{x},z+\frac{1}{2}$	$0kl$: $k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y,\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x,\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
8	h	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},0$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	
8	g	. . 2	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	hkl: $l=2n$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	
8	f	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{2}$	
8	e	2 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $h+k,l=2n$
			$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	
4	d	2 . 2 2	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	hkl: $h+k,l=2n$
4	c	$2/m$ . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h+k,l=2n$
4	b	$\bar{4}$ . .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	hkl: $h+k,l=2n$
4	a	$2/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k,l=2n$

Symmetry of special projections

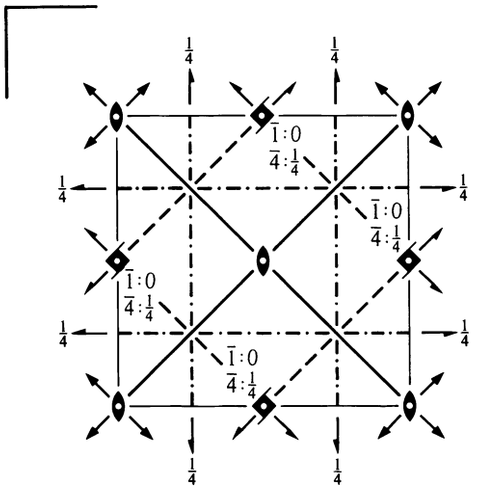
Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

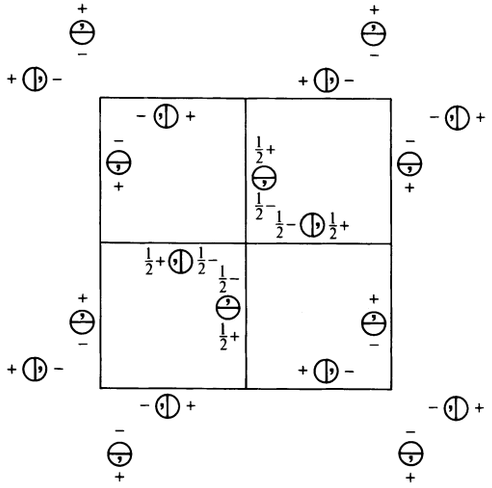
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4_2/mnm$ D_{4h}^{14} $4/mmm$ Tetragonal

No. 136 $P\ 4_2/m\ 2_1/n\ 2/m$ Patterson symmetry $P4/mmm$





Origin at centre (mmm) at $2/m\,1\,2/m$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},\frac{1}{4}$	(7) $2\ \ x,x,0$	(8) $2\ \ x,\bar{x},0$
(9) $\bar{1}\ \ 0,0,0$	(10) $m\ \ x,y,0$	(11) $\bar{4}^+\ \frac{1}{2},0,z;\ \ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-\ 0,\frac{1}{2},z;\ \ 0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,z$	(15) $m\ \ x,\bar{x},z$	(16) $m\ \ x,x,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z	
							Special: as above, plus
8	j	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	i	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y,x,0$	$\bar{y},\bar{x},0$	
8	h	$2..$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	hkl: $h+k,l=2n$
			$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$	
4	g	$m.2m$	$x,\bar{x},0$	$\bar{x},x,0$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	f	$m.2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	e	$2.mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	hkl: $h+k+l=2n$
4	d	$\bar{4}..$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k,l=2n$
4	c	$2/m..$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$	hkl: $h+k,l=2n$
2	b	$m.mm$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $h+k+l=2n$
2	a	$m.mm$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

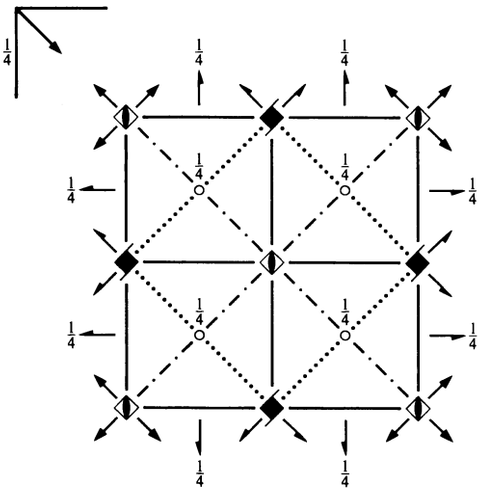
Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

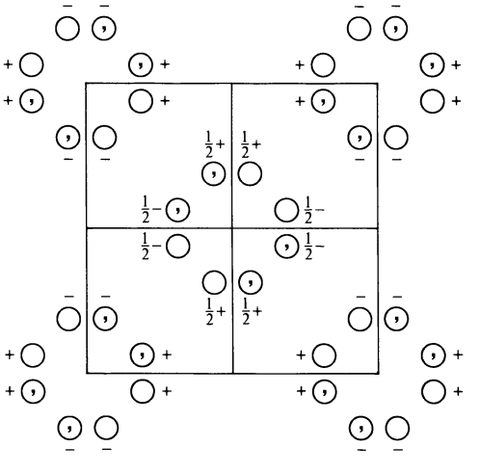
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$P4_2/nmc$ D_{4h}^{15} $4/mmm$ Tetragonal

No. 137 $P\ 4_2/n\ 2_1/m\ 2/c$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2/n$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) m $x,0,z$	(14) m $0,y,z$	(15) c $x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	hhl: $l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
			(13) $x,\bar{y},z$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$h00$: $h=2n$
							Special: as above, plus
8	g	$.m.$	$0,y,z$	$0,\bar{y},z$	$\bar{y}+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	
8	f	$..2$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x,\bar{x},0$	$\bar{x},x,0$	
8	e	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	hkl: $h,k,l=2n$
4	d	$2\,m\,m.$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$					hkl: $l=2n$
4	c	$2\,m\,m.$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$					hkl: $h+k+l=2n$
2	b	$\bar{4}\,m\,2$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$							hkl: $h+k+l=2n$
2	a	$\bar{4}\,m\,2$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$							hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

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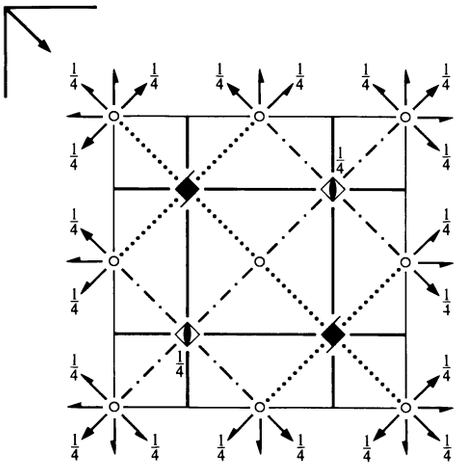
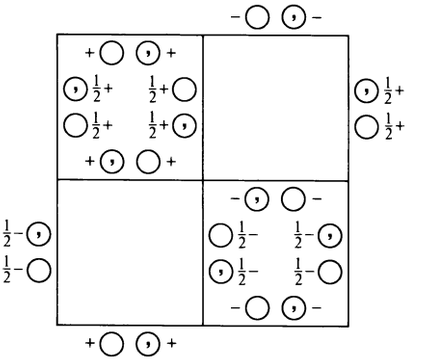
Patterson symmetry $P4/mmm$

$P\ 4_2/n\ 2_1/m\ 2/c$ No. 137

ORIGIN CHOICE 2





Origin at $\bar{1}$ at $n2_1(c,n)$, at $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$ from $\bar{4}m2$

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{4};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{4}$

Symmetry operations

(1) 1	(2) $2\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)\ \ 0,y,0$	(6) $2(\frac{1}{2},0,0)\ \ x,0,0$	(7) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x,\frac{1}{4}$	(8) $2\ \ x,\bar{x},\frac{1}{4}$
(9) $\bar{1}\ \ 0,0,0$	(10) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$	(11) $\bar{4}^+\ \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(12) $\bar{4}^-\ -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(13) $m\ \ x,\frac{1}{4},z$	(14) $m\ \ \frac{1}{4},y,z$	(15) $c\ \ x+\frac{1}{2},\bar{x},z$	(16) $c\ \ x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											General:
16	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$					$hk0$: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$					hhl: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$					$00l$: $l=2n$
			(13) $x,\bar{y}+\frac{1}{2},z$	(14) $\bar{x}+\frac{1}{2},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $y,x,z+\frac{1}{2}$					$h00$: $h=2n$
											Special: as above, plus
8	g	$.m.$	$\frac{1}{4},y,z$	$\frac{1}{4},\bar{y}+\frac{1}{2},z$	$\bar{y}+\frac{1}{2},\frac{1}{4},z+\frac{1}{2}$	$y,\frac{1}{4},z+\frac{1}{2}$					no extra conditions
			$\frac{3}{4},y+\frac{1}{2},\bar{z}$	$\frac{3}{4},\bar{y},\bar{z}$	$y+\frac{1}{2},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\bar{y},\frac{3}{4},\bar{z}+\frac{1}{2}$					
8	f	$..2$	$x,\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$					hkl: $h+k+l=2n$
			$\bar{x},x,\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\bar{x},\frac{1}{4}$	$x,x+\frac{1}{2},\frac{1}{4}$					
8	e	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	hkl: $h,k,l=2n$
4	d	$2\,m\,m.$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$					hkl: $l=2n$
4	c	$2\,m\,m.$	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$					hkl: $h+k+l=2n$
2	b	$\bar{4}\,m\,2$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$							hkl: $h+k+l=2n$
2	a	$\bar{4}\,m\,2$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$							hkl: $h+k+l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

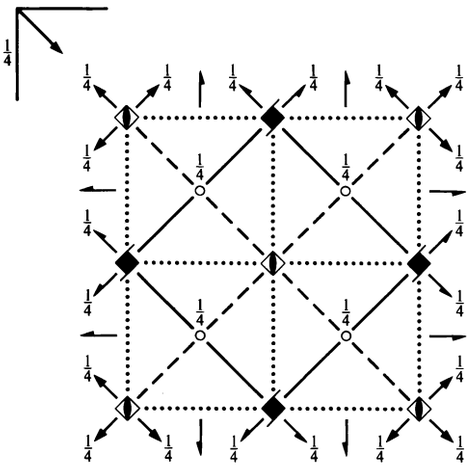
Along [100] $p2mg$
$\mathbf{a}'=\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

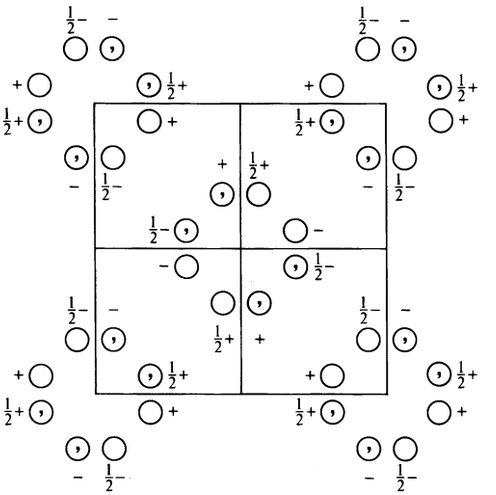
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\quad \mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4_2/ncm$ D_{4h}^{16} $4/mmm$ Tetragonal

No. 138 $P\ 4_2/n\ 2_1/c\ 2/m$ Patterson symmetry $P4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}c\,g$, at $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le y$; $y \le \frac{1}{2} - x$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},\frac{1}{4}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) c $x,0,z$	(14) c $0,y,z$	(15) m $x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$0kl$: $l=2n$
			(9) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y},x,\bar{z}$	$00l$: $l=2n$
			(13) $x,\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) $y+\frac{1}{2},x+\frac{1}{2},z$	$h00$: $h=2n$
							Special: as above, plus
8	i	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x},x+\frac{1}{2},z+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x}+\frac{1}{2},x,\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}$	$x+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	
8	h	$..2$	$x,x,\frac{3}{4}$	$\bar{x},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{1}{4}$	
8	g	$..2$	$x,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	hkl: $h+k=2n$
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	$x,\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	
8	f	$2..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$	hkl: $h+k,l=2n$
			$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z$	
4	e	$2.mm$	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
4	d	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$
4	c	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
4	b	$\bar{4}..$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,0,\frac{1}{2}$	hkl: $h+k,l=2n$
4	a	2.22	$0,0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$0,0,\frac{3}{4}$	hkl: $h+k,l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

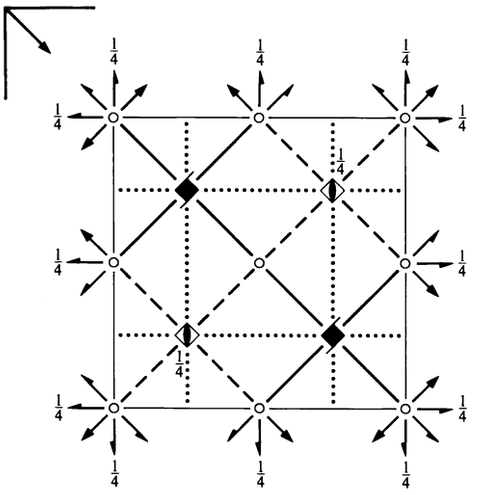
Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{4},0$

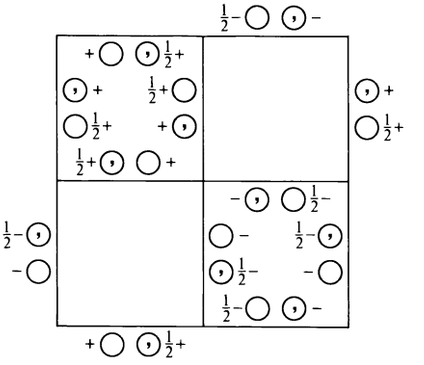
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

No. 138 $P\ 4_2/n\ 2_1/c\ 2/m$

Patterson symmetry $P4/mmm$

ORIGIN CHOICE 2





Origin at centre $(2/m)$ at $n\,1\,(2/m, 2_1/g)$, at $\frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$ from $\bar{4}$

Asymmetric unit $-\frac{1}{4} \le x \le \frac{1}{4}; \quad -\frac{1}{4} \le y \le \frac{1}{4}; \quad 0 \le z \le \frac{1}{2}; \quad x \le y$

Symmetry operations

(1) 1
(2) $2 \quad \frac{1}{4}, \frac{1}{4}, z$
(3) $4^+(0,0,\frac{1}{2}) \quad \frac{1}{4}, \frac{1}{4}, z$
(4) $4^-(0,0,\frac{1}{2}) \quad \frac{1}{4}, \frac{1}{4}, z$
(5) $2(0,\frac{1}{2},0) \quad 0, y, \frac{1}{4}$
(6) $2(\frac{1}{2},0,0) \quad x, 0, \frac{1}{4}$
(7) $2(\frac{1}{2},\frac{1}{2},0) \quad x, x, 0$
(8) $2 \quad x, \bar{x}, 0$
(9) $\bar{1} \quad 0,0,0$
(10) $n(\frac{1}{2},\frac{1}{2},0) \quad x, y, 0$
(11) $\bar{4}^+ \quad \frac{1}{4}, -\frac{1}{4}, z; \quad \frac{1}{4}, -\frac{1}{4}, \frac{1}{4}$
(12) $\bar{4}^- \quad -\frac{1}{4}, \frac{1}{4}, z; \quad -\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
(13) $c \quad x, \frac{1}{4}, z$
(14) $c \quad \frac{1}{4}, y, z$
(15) $m \quad x + \frac{1}{2}, \bar{x}, z$
(16) $m \quad x, x, z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
16	j	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{y}+\frac{1}{2},x,z+\frac{1}{2}$	(4) $y,\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h+k=2n$
			(5) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$	$0kl$: $l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(11) $y+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	(12) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$00l$: $l=2n$
			(13) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(16) y,x,z	$h00$: $h=2n$
							Special: as above, plus
8	i	. . m	x,x,z	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},z+\frac{1}{2}$	no extra conditions
			$\bar{x},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
8	h	. . 2	$x,\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},0$	$x+\frac{1}{2},x,\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{2}$	hkl: $h+k=2n$
			$\bar{x},x,0$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},\bar{x},\frac{1}{2}$	$x,x+\frac{1}{2},\frac{1}{2}$	
8	g	. . 2	$x,\bar{x},\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},x,0$	$\bar{x},\bar{x}+\frac{1}{2},0$	hkl: $h+k=2n$
			$\bar{x},x,\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x},0$	$x,x+\frac{1}{2},0$	
8	f	2 . .	$\frac{3}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{z}$	hkl: $h+k,l=2n$
			$\frac{1}{4},\frac{3}{4},\bar{z}$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},z$	
4	e	2 . mm	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{1}{4},z+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	hkl: $l=2n$
4	d	. . 2/m	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
4	c	. . 2/m	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	hkl: $h+k,h+l,k+l=2n$
4	b	$\bar{4}$ . .	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h+k,l=2n$
4	a	2 . 2 2	$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	hkl: $h+k,l=2n$

Symmetry of special projections

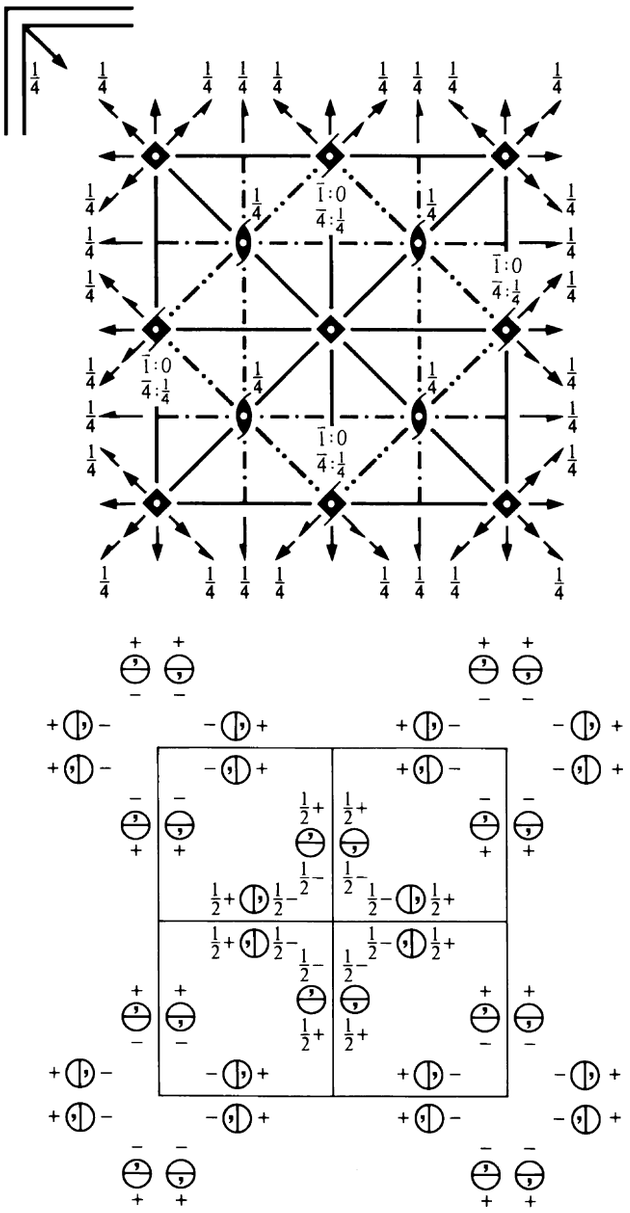
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [100] $p2mg$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$I4/mmm$ D_{4h}^{17} $4/mmm$ Tetragonal

No. 139 $I\ 4/m\ 2/m\ 2/m$ Patterson symmetry $I4/mmm$



Origin at centre $(4/mmm)$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}; \quad x \le y$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,0$	(6) 2 $x,0,0$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $0,0,0$	(10) m $x,y,0$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) m $x,0,z$	(14) m $0,y,z$	(15) m $x,\bar{x},z$	(16) m x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(15) c $x+\frac{1}{2},\bar{x},z$	(16) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	o	1	(1) x,y,z (5) $\bar{x},y,\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (14) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}$ (12) $\bar{y},x,\bar{z}$ (16) y,x,z	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
16	n	. m .	$0,y,z$ $0,y,\bar{z}$	$0,\bar{y},z$ $0,\bar{y},\bar{z}$	$\bar{y},0,z$ $y,0,\bar{z}$	$y,0,z$ $\bar{y},0,\bar{z}$	no extra conditions
16	m	. . m	x,x,z $\bar{x},x,\bar{z}$	$\bar{x},\bar{x},z$ $x,\bar{x},\bar{z}$	$\bar{x},x,z$ $x,x,\bar{z}$	$x,\bar{x},z$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
16	l	m . .	$x,y,0$ $\bar{x},y,0$	$\bar{x},\bar{y},0$ $x,\bar{y},0$	$\bar{y},x,0$ $y,x,0$	$y,\bar{x},0$ $\bar{y},\bar{x},0$	no extra conditions
16	k	. . 2	$x,x+\frac{1}{2},\frac{1}{4}$ $\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$ $x,x+\frac{1}{2},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$ $x+\frac{1}{2},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$ $\bar{x}+\frac{1}{2},x,\frac{3}{4}$	hkl: $l=2n$
8	j	m 2 m .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	no extra conditions
8	i	m 2 m .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	no extra conditions
8	h	m . 2 m	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$	no extra conditions
8	g	2 m m .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	hkl: $l=2n$
8	f	. . 2/m	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl: $k,l=2n$
4	e	4 m m	$0,0,z$	$0,0,\bar{z}$			no extra conditions
4	d	$\bar{4}$ m 2	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl: $l=2n$
4	c	m m m .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $l=2n$
2	b	4/m m m	$0,0,\frac{1}{2}$				no extra conditions
2	a	4/m m m	$0,0,0$				no extra conditions

Symmetry of special projections

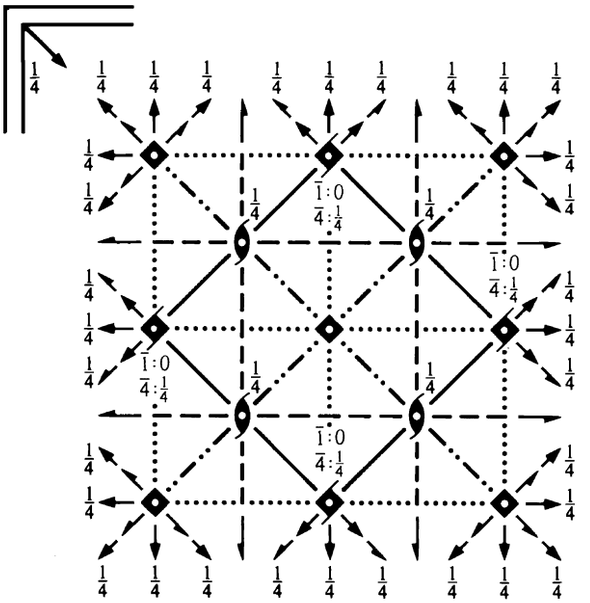
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

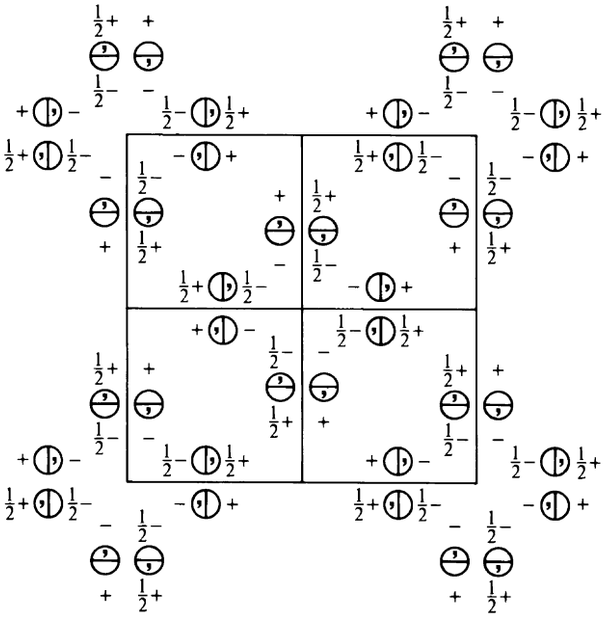
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$I4/mcm$ D_{4h}^{18} $4/mmm$ Tetragonal

No. 140 $I\ 4/m\ 2/c\ 2/m$ Patterson symmetry $I4/mmm$





Origin at centre $(4/m)$ at $4/mc2_1/e$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $y \le \frac{1}{2} - x$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) 2 $0,y,\frac{1}{4}$	(6) 2 $x,0,\frac{1}{4}$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},\frac{1}{4}$
(9) $\bar{1}$ $0,0,0$	(10) m $x,y,0$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) c $x,0,z$	(14) c $0,y,z$	(15) c $x,\bar{x},z$	(16) c x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(13) a $x,\frac{1}{4},z$	(14) b $\frac{1}{4},y,z$	(15) m $x+\frac{1}{2},\bar{x},z$	(16) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	m	1	(1) x,y,z (5) $\bar{x},y,\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{y},\bar{z}$ (13) $x,\bar{y},z+\frac{1}{2}$	(2) $\bar{x},\bar{y},z$ (6) $x,\bar{y},\bar{z}+\frac{1}{2}$ (10) $x,y,\bar{z}$ (14) $\bar{x},y,z+\frac{1}{2}$	(3) $\bar{y},x,z$ (7) $y,x,\bar{z}+\frac{1}{2}$ (11) $y,\bar{x},\bar{z}$ (15) $\bar{y},\bar{x},z+\frac{1}{2}$	(4) $y,\bar{x},z$ (8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (12) $\bar{y},x,\bar{z}$ (16) $y,x,z+\frac{1}{2}$	hkl: $h+k+l=2n$ $hk0$: $h+k=2n$ $0kl$: $k,l=2n$ hhl: $l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
							Special: as above, plus
16	l	$..m$	$x,x+\frac{1}{2},z$ $\bar{x},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2},z$ $x,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,z$ $x+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x},z$ $\bar{x}+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	no extra conditions
16	k	$m..$	$x,y,0$ $\bar{x},y,\frac{1}{2}$	$\bar{x},\bar{y},0$ $x,\bar{y},\frac{1}{2}$	$\bar{y},x,0$ $y,x,\frac{1}{2}$	$y,\bar{x},0$ $\bar{y},\bar{x},\frac{1}{2}$	no extra conditions
16	j	$.2.$	$x,0,\frac{1}{4}$ $\bar{x},0,\frac{3}{4}$	$\bar{x},0,\frac{1}{4}$ $x,0,\frac{3}{4}$	$0,x,\frac{1}{4}$ $0,\bar{x},\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$ $0,x,\frac{3}{4}$	hkl: $l=2n$
16	i	$..2$	$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},\bar{x},\frac{1}{4}$ $x,x,\frac{3}{4}$	$\bar{x},x,\frac{1}{4}$ $x,\bar{x},\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{3}{4}$	hkl: $l=2n$
8	h	$m.2m$	$x,x+\frac{1}{2},0$	$\bar{x},\bar{x}+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},x,0$	$x+\frac{1}{2},\bar{x},0$	no extra conditions
8	g	$2.mm$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	hkl: $l=2n$
8	f	$4..$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	e	$..2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl: $k,l=2n$
4	d	$m.mm$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $l=2n$
4	c	$4/m..$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
4	b	$\bar{4}\,2\,m$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$			hkl: $l=2n$
4	a	$4\,2\,2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

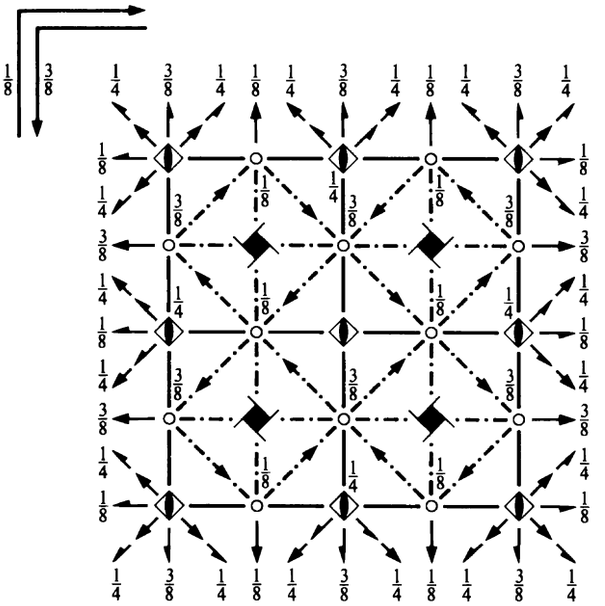
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

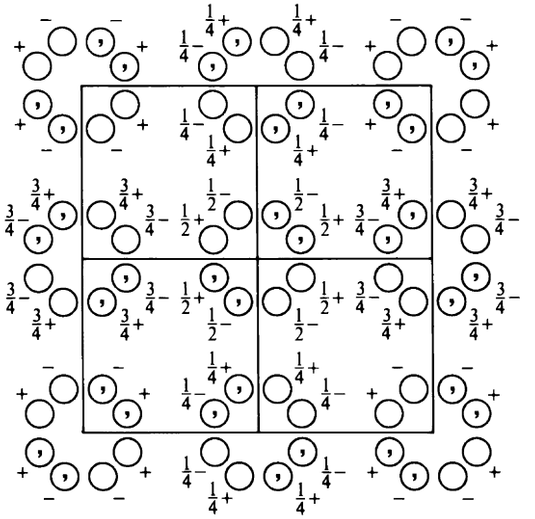
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$I4_1/amd$ D_{4h}^{19} $4/mmm$ Tetragonal

No. 141 $I\ 4_1/a\ 2/m\ 2/d$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1





Origin at $\bar{4}m2$, at $0,\frac{1}{4},-\frac{1}{8}$ from centre $(2/m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,\frac{3}{8}$	(6) 2 $x,\frac{1}{4},\frac{1}{8}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x},0$
(9) $\bar{1}$ $0,\frac{1}{4},\frac{1}{8}$	(10) a $x,y,\frac{3}{8}$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(14) m $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x-\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{8}$	(6) $2(\frac{1}{2},0,0)$ $x,0,\frac{3}{8}$	(7) 2 $x,x,0$	(8) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(9) $\bar{1}$ $\frac{1}{4},0,\frac{3}{8}$	(10) b $x,y,\frac{1}{8}$	(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) m $x,0,z$	(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},x,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl: $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl: $2h+l=4n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(8) $\bar{y},\bar{x},\bar{z}$	
			(9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{3}{4}$	(16) $y,x+\frac{1}{2},z+\frac{1}{4}$	
							Special: as above, plus
16	h	. m .	$0,y,z$	$\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$\bar{y},\frac{1}{2},z+\frac{1}{4}$	$y+\frac{1}{2},0,z+\frac{3}{4}$	no extra conditions
			$\frac{1}{2},y,\bar{z}+\frac{3}{4}$	$0,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	$y+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{y},0,\bar{z}$	
16	g	. . 2	$x,x,0$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	hkl: $l=2n+1$ or $2h+l=4n$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x+\frac{1}{2},x,\frac{3}{4}$	$x,\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	
16	f	. 2 .	$x,\frac{1}{4},\frac{1}{8}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},\bar{x},\frac{7}{8}$	hkl: $l=2n+1$ or $h=2n$
			$\bar{x},\frac{1}{4},\frac{1}{8}$	$x+\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{1}{4},\bar{x},\frac{7}{8}$	$\frac{1}{4},x+\frac{1}{2},\frac{3}{8}$	
8	e	2 m m .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	hkl: $l=2n+1$ or $2h+l=4n$
8	d	. $2/m$.	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$	hkl: $l=2n+1$ or $h,k=2n$, $h+k+l=4n$
8	c	. $2/m$.	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$	
4	b	$\bar{4}$ m 2	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}$ m 2	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$			

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

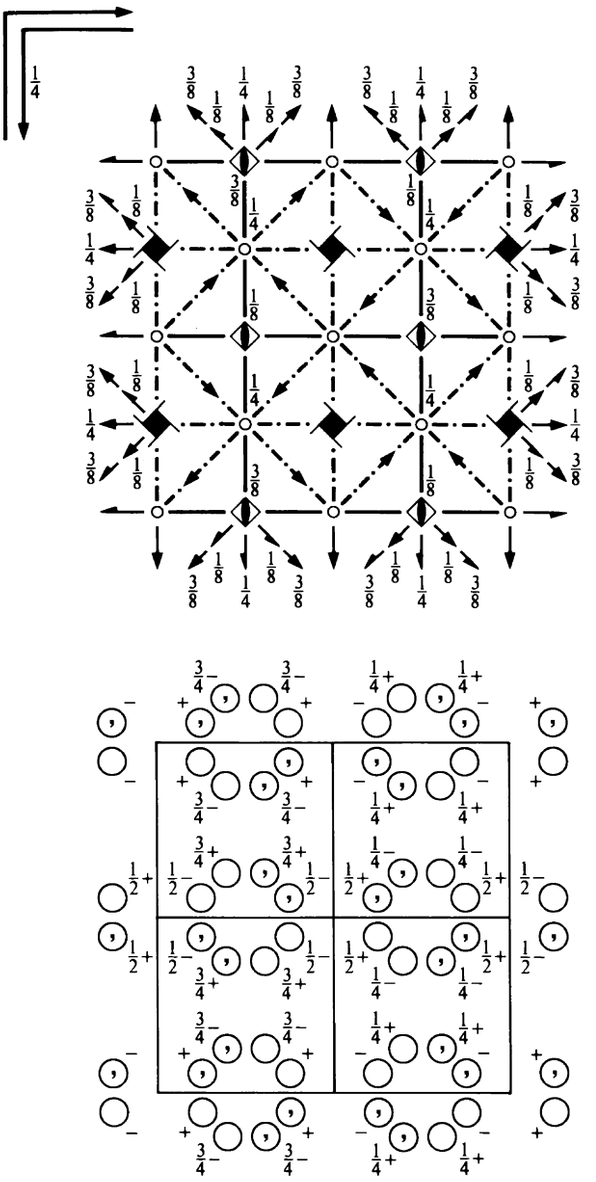
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{3}{8}$

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

No. 141 $I\ 4_1/a\ 2/m\ 2/d$

Patterson symmetry $I4/mmm$

ORIGIN CHOICE 2



Origin at centre $(2/m)$ at $b\,(2/m,2_1/n)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}m2$

Asymmetric unit $0\le x\le\frac{1}{2};\quad -\frac{1}{4}\le y\le\frac{1}{4};\quad 0\le z\le\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(5) 2 $\frac{1}{4},y,\frac{1}{4}$	(6) 2 $x,0,0$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{1}{8}$	(8) 2 $x,\bar{x}+\frac{1}{4},\frac{3}{8}$
(9) $\bar{1}$ $0,0,0$	(10) a $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z;$ $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^-$ $0,\frac{3}{4},z;$ $0,\frac{3}{4},\frac{1}{8}$
(13) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(14) m $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{1}{4})$ x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)$ $0,y,0$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$	(8) 2 $x,\bar{x}+\frac{3}{4},\frac{1}{8}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) b $x,y,0$	(11) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z;$ $\frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^-$ $0,\frac{1}{4},z;$ $0,\frac{1}{4},\frac{3}{8}$
(13) m $x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	(4) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	hkl: $h+k+l=2n$ $hk0$: $h,k=2n$ $0kl$: $k+l=2n$ hhl: $2h+l=4n$ $00l$: $l=4n$ $h00$: $h=2n$ $h\bar{h}0$: $h=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(6) $x,\bar{y},\bar{z}$	(7) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	(8) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(11) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	
			(13) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(14) $\bar{x},y,z$	(15) $\bar{y}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $y+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	
							Special: as above, plus
16	h	. m .	$0,y,z$	$\frac{1}{2},\bar{y},z+\frac{1}{2}$	$\bar{y}+\frac{1}{4},\frac{3}{4},z+\frac{1}{4}$	$y+\frac{1}{4},\frac{1}{4},z+\frac{3}{4}$	no extra conditions
			$\frac{1}{2},y,\bar{z}+\frac{1}{2}$	$0,\bar{y},\bar{z}$	$y+\frac{1}{4},\frac{3}{4},\bar{z}+\frac{1}{4}$	$\bar{y}+\frac{1}{4},\frac{1}{4},\bar{z}+\frac{3}{4}$	
16	g	. . 2	$x,x+\frac{1}{4},\frac{7}{8}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{3}{4},\frac{3}{8}$	$\bar{x},x+\frac{3}{4},\frac{1}{8}$	$x+\frac{1}{2},\bar{x}+\frac{1}{4},\frac{5}{8}$	hkl: $l=2n+1$ or $2h+l=4n$
			$\bar{x},\bar{x}+\frac{3}{4},\frac{1}{8}$	$x+\frac{1}{2},x+\frac{1}{4},\frac{5}{8}$	$x,\bar{x}+\frac{1}{4},\frac{7}{8}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},\frac{3}{8}$	
16	f	. 2 .	$x,0,0$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{4},x+\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{3}{4}$	hkl: $l=2n+1$ or $h=2n$
			$\bar{x},0,0$	$x+\frac{1}{2},0,\frac{1}{2}$	$\frac{3}{4},\bar{x}+\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},x+\frac{3}{4},\frac{1}{4}$	
8	e	2 m m	$0,\frac{1}{4},z$	$0,\frac{3}{4},z+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{1}{4}$	hkl: $l=2n+1$ or $2h+l=4n$
8	d	. $2/m$.	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	hkl: $l=2n+1$ or $h,k=2n$, $h+k+l=4n$
8	c	. $2/m$.	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	
4	b	$\bar{4}$ m 2	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{5}{8}$			hkl: $l=2n+1$ or $2h+l=4n$
4	a	$\bar{4}$ m 2	$0,\frac{3}{4},\frac{1}{8}$	$\frac{1}{2},\frac{3}{4},\frac{3}{8}$			

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4},0,z$

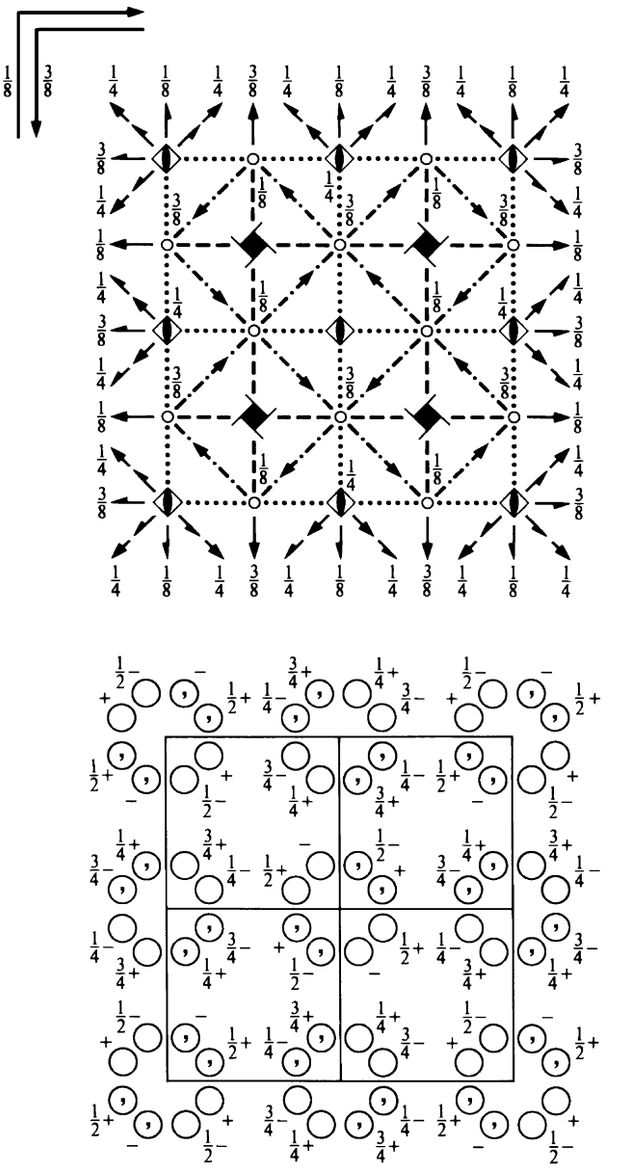
Along [100] $c2mm$
$\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{1}{8}$

$I4_1/acd$ D_{4h}^{20} $4/mmm$ Tetragonal

No. 142 $I\ 4_1/a\ 2/c\ 2/d$ Patterson symmetry $I4/mmm$

ORIGIN CHOICE 1



Origin at $\bar{4}c2_1$, at $0,\frac{1}{4},-\frac{1}{8}$ from $\bar{1}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},-\frac{1}{4},z$
(5) 2 $\frac{1}{4},y,\frac{1}{8}$	(6) 2 $x,\frac{1}{4},\frac{3}{8}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$	(8) 2 $x,\bar{x},\frac{1}{4}$
(9) $\bar{1}$ $0,\frac{1}{4},\frac{1}{8}$	(10) a $x,y,\frac{3}{8}$	(11) $\bar{4}^+$ $0,0,z$; $0,0,0$	(12) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(13) a $x,\frac{1}{4},z$	(14) c $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x-\frac{1}{4},x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,0,z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{4},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},\frac{1}{4},z$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{3}{8}$	(6) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{8}$	(7) 2 $x,x,\frac{1}{4}$	(8) 2 $x,\bar{x}+\frac{1}{2},0$
(9) $\bar{1}$ $\frac{1}{4},0,\frac{3}{8}$	(10) b $x,y,\frac{1}{8}$	(11) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-$ $0,0,z$; $0,0,0$
(13) c $x,0,z$	(14) b $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{4},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},x,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							General:
32	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{y},x+\frac{1}{2},z+\frac{1}{4}$	(4) $y+\frac{1}{2},\bar{x},z+\frac{3}{4}$	hkl: $h+k+l=2n$
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{4}$	(6) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{3}{4}$	(7) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	$hk0$: $h,k=2n$
			(9) $\bar{x},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{4}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{3}{4}$	(11) $y,\bar{x},\bar{z}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k,l=2n$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{4}$	(16) $y,x+\frac{1}{2},z+\frac{3}{4}$	hhl: $2h+l=4n$
							$00l$: $l=4n$
							$h00$: $h=2n$
							$h\bar{h}0$: $h=2n$
							Special: as above, plus
16	f	. . 2	$x,x,\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\bar{x},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x},0$	hkl: $l=2n+1$
			$\bar{x},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},x,\frac{1}{2}$	$x,\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{4}$	or $2h+l=4n$
16	e	. 2 .	$\frac{1}{4},y,\frac{1}{8}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\frac{5}{8}$	$\bar{y},\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},\frac{3}{4},\frac{7}{8}$	hkl: $l=2n+1$
			$\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{8}$	$\frac{3}{4},y,\frac{5}{8}$	$y,\frac{3}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},\frac{3}{4},\frac{3}{8}$	or $h=2n$
16	d	2 . .	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	hkl: $2h+l=4n$
			$0,\frac{1}{2},\bar{z}+\frac{1}{4}$	$0,0,\bar{z}$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{4}$	
16	c	$\bar{1}$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$	hkl: $h,k=2n,\ h+k+l=4n$
8	b	2 . 2 2	$0,0,\frac{1}{4}$	$0,\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$0,0,\frac{3}{4}$					hkl: $2h+l=4n$
8	a	$\bar{4}$ . .	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},0$					hkl: $2h+l=4n$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

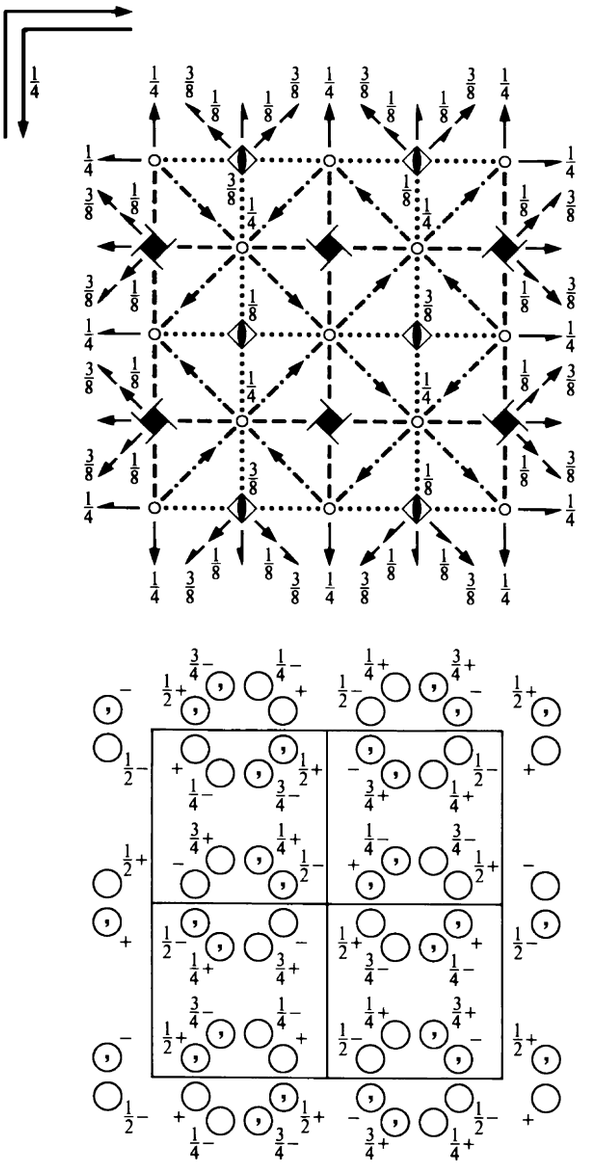
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,\frac{1}{8}$

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

No. 142 $I\ 4_1/a\ 2/c\ 2/d$

Patterson symmetry $I4/mmm$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $b(c,a)d$, at $0,-\frac{1}{4},\frac{1}{8}$ from $\bar{4}$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(5) 2 $\frac{1}{4},y,0$	(6) 2 $x,0,\frac{1}{4}$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$	(8) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(9) $\bar{1}$ $0,0,0$	(10) a $x,y,\frac{1}{4}$	(11) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$	(12) $\bar{4}^-$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
(13) a $x,0,z$	(14) c $0,y,z$	(15) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,x,z

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(5) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$	(7) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$	(8) 2 $x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(9) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(10) b $x,y,0$	(11) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$	(12) $\bar{4}^-$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
(13) c $x,\frac{1}{4},z$	(14) b $\frac{1}{4},y,z$	(15) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$	(16) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,x,z

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
32	g	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	(4) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	General:
			(5) $\bar{x}+\frac{1}{2},y,\bar{z}$	(6) $x,\bar{y},\bar{z}+\frac{1}{2}$	(7) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{3}{4}$	(8) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	hkl: $h+k+l=2n$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(11) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	$hk0$: $h,k=2n$
			(13) $x+\frac{1}{2},\bar{y},z$	(14) $\bar{x},y,z+\frac{1}{2}$	(15) $\bar{y}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{4}$	(16) $y+\frac{3}{4},x+\frac{3}{4},z+\frac{3}{4}$	$0kl$: $k,l=2n$
							hhl: $2h+l=4n$
							$00l$: $l=4n$
							$h\bar{h}0$: $h=2n$
							Special: as above, plus
16	f	. . 2	$x,x+\frac{1}{4},\frac{1}{8}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{3}{4},\frac{5}{8}$	$\bar{x},x+\frac{3}{4},\frac{3}{8}$	$x+\frac{1}{2},\bar{x}+\frac{1}{4},\frac{7}{8}$	hkl: $l=2n+1$
			$\bar{x},\bar{x}+\frac{3}{4},\frac{7}{8}$	$x+\frac{1}{2},x+\frac{1}{4},\frac{3}{8}$	$x,\bar{x}+\frac{1}{4},\frac{5}{8}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},\frac{1}{8}$	or $2h+l=4n$
16	e	. 2 .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x+\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\bar{x}+\frac{1}{4},0$	hkl: $l=2n+1$
			$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},x+\frac{3}{4},0$	or $h=2n$
16	d	2 . .	$0,\frac{1}{4},z$	$0,\frac{3}{4},z+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\bar{z}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{3}{4}$	hkl: $2h+l=4n$
			$0,\frac{3}{4},\bar{z}$	$0,\frac{1}{4},\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},z$	$\frac{1}{2},\frac{1}{4},z+\frac{1}{4}$	
16	c	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},0,0$ $0,0,\frac{1}{2}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h,k=2n,\ h+k+l=4n$
8	b	2 . 2 2	$0,\frac{1}{4},\frac{1}{8}$	$0,\frac{3}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{7}{8}$	$0,\frac{1}{4},\frac{5}{8}$	hkl: $2h+l=4n$
8	a	$\bar{4}$ . .	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{3}{4},\frac{3}{8}$	hkl: $2h+l=4n$

Symmetry of special projections

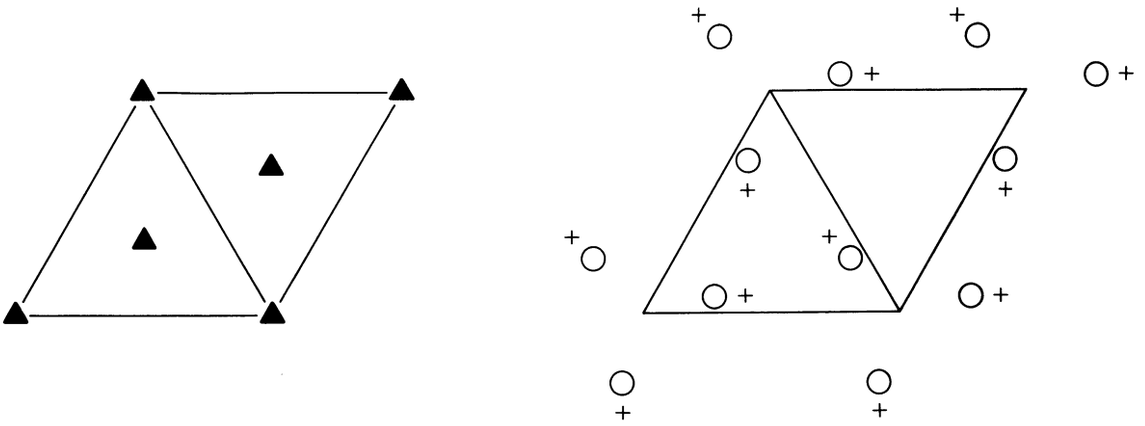
Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{1}{8}$

$P3$ C_3^1 3 Trigonal

No. 143 $P3$ Patterson symmetry $P\bar{3}$



Origin on 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$ $\frac{1}{3},\frac{2}{3},1$ $0,\frac{1}{2},1$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
3	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
						Special: no extra conditions
1	c	3 . .	$\frac{2}{3},\frac{1}{3},z$			
1	b	3 . .	$\frac{1}{3},\frac{2}{3},z$			
1	a	3 . .	$0,0,z$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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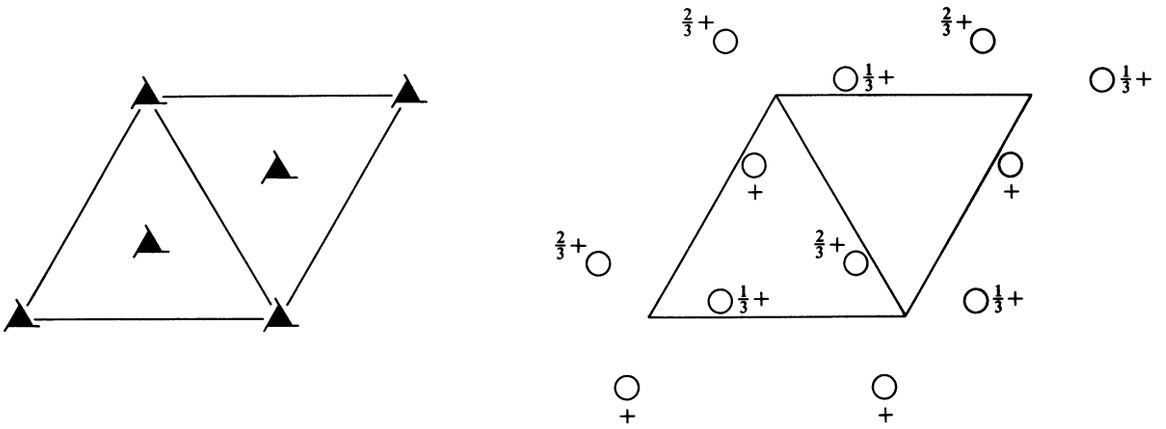
Trigonal 3 C_3^2 $P3_1$

Patterson symmetry $P\bar{3}$ $P3_1$ No. 144



Origin on 3_1

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{3}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$
$0,0,\frac{1}{3} \quad 1,0,\frac{1}{3} \quad 1,1,\frac{1}{3} \quad 0,1,\frac{1}{3}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
3 a 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l: l = 3n$

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

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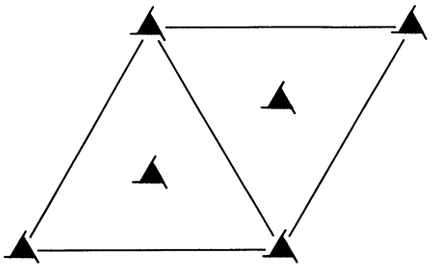
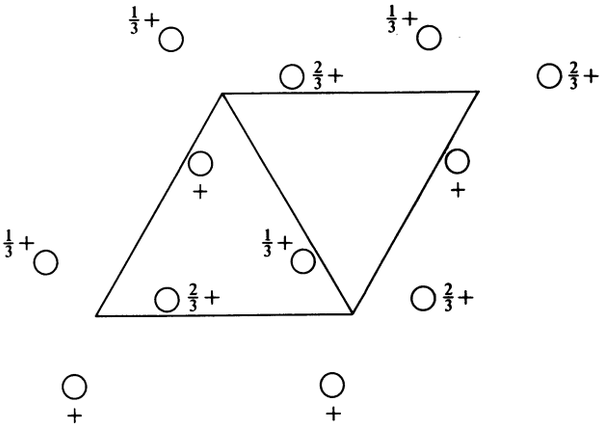
$P3_2$ C_3^3 3 Trigonal

No. 145 $P3_2$ Patterson symmetry $P\bar{3}$





Origin on 3_2

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{3}$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0\quad 0,1,0$
$0,0,\frac{1}{3}\quad 1,0,\frac{1}{3}\quad 1,1,\frac{1}{3}\quad 0,1,\frac{1}{3}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
3 a 1	(1) x,y,z (2) $\bar{y},x-y,z+\frac{2}{3}$ (3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l: l = 3n$

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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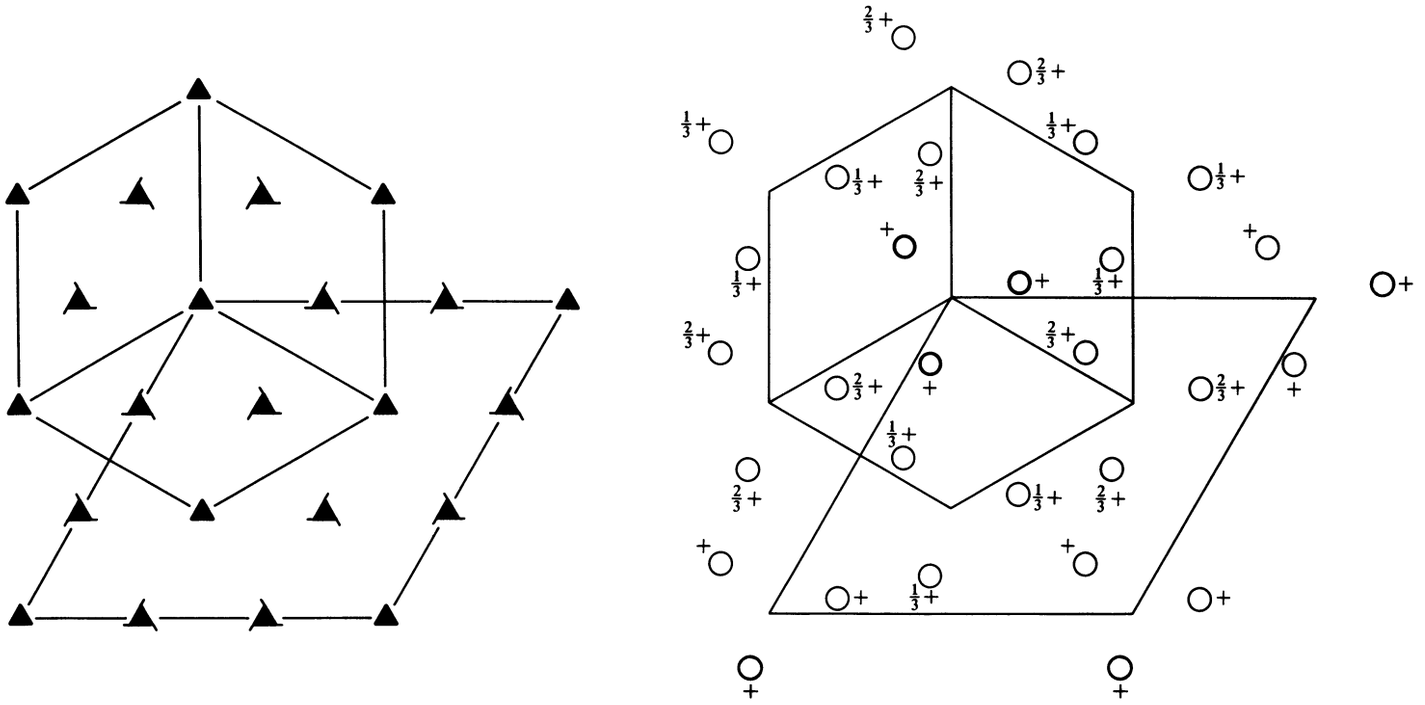
Trigonal 3 C_3^4 $R3$

Patterson symmetry $R\bar{3}$ $R3$ No. 146

HEXAGONAL AXES



Origin on 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{3}$ $\frac{1}{2},0,\frac{1}{3}$ $\frac{2}{3},\frac{1}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3},\frac{1}{3}$ $0,\frac{1}{2},\frac{1}{3}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ (2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$ (3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ (2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$ (3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
	$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	
9 *b* 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	General:
				$hkil$: $-h+k+l=3n$
				$hki0$: $-h+k=3n$
				$hh\overline{2h}l$: $l=3n$
				$h\bar{h}0l$: $h+l=3n$
				$000l$: $l=3n$
				$h\bar{h}00$: $h=3n$
				Special: no extra conditions
3 *a* 3.	$0,0,z$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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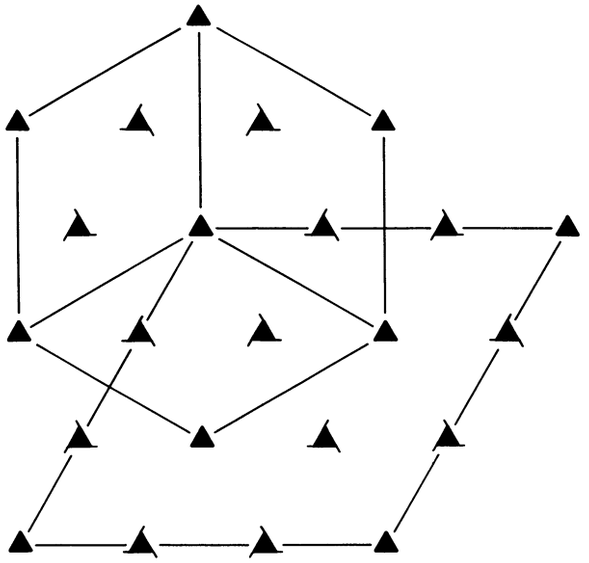
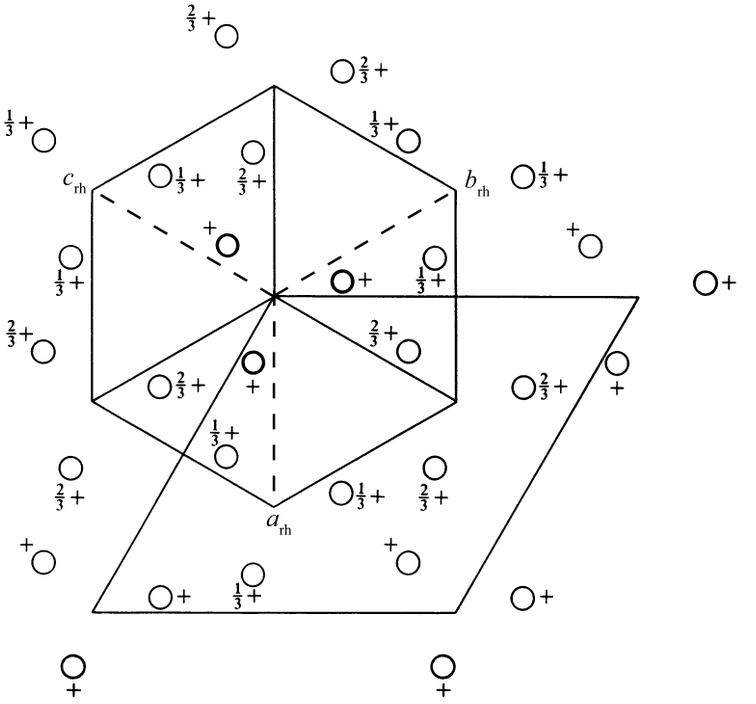




Heights refer to hexagonal axes

Origin on 3

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le 1;\quad z \le \min(x,y)$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0\quad 0,1,0\quad 1,1,1$

Symmetry operations

(1) 1 (2) 3^+ x,x,x (3) 3^- x,x,x

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
3 b 1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
				Special: no extra conditions
1 a 3 .	x,x,x			

Symmetry of special projections

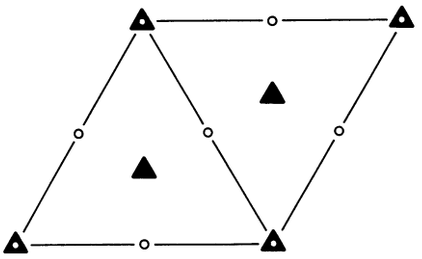
Along [111] $p3$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

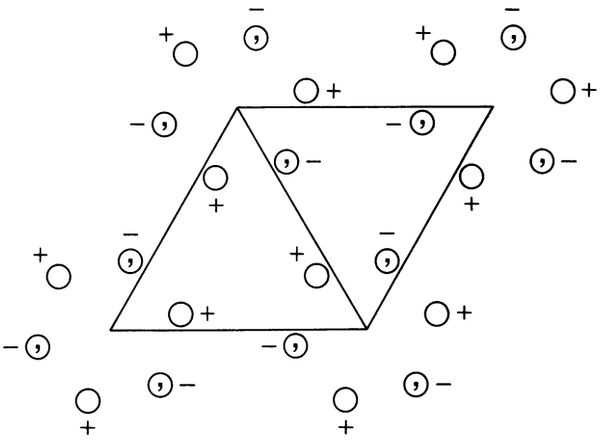
Along [1$\bar{1}$0] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along [2$\bar{1}\bar{1}$] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

Trigonal $\bar{3}$ C_{3i}^{1} $P\bar{3}$

Patterson symmetry $P\bar{3}$ $P\bar{3}$ No. 147





Origin at centre $(\bar{3})$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) $\bar{1}$ $0,0,0$ (5) $\bar{3}^+$ $0,0,z$; $0,0,0$ (6) $\bar{3}^-$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{x},\bar{y},\bar{z}$	(5) $y,\bar{x}+y,\bar{z}$	(6) $x-y,x,\bar{z}$	
						Special: no extra conditions
3	f	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
3	e	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
2	d	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	c	$3\,.\,.$	$0,0,z$	$0,0,\bar{z}$		
1	b	$\bar{3}\,.\,.$	$0,0,\frac{1}{2}$			
1	a	$\bar{3}\,.\,.$	$0,0,0$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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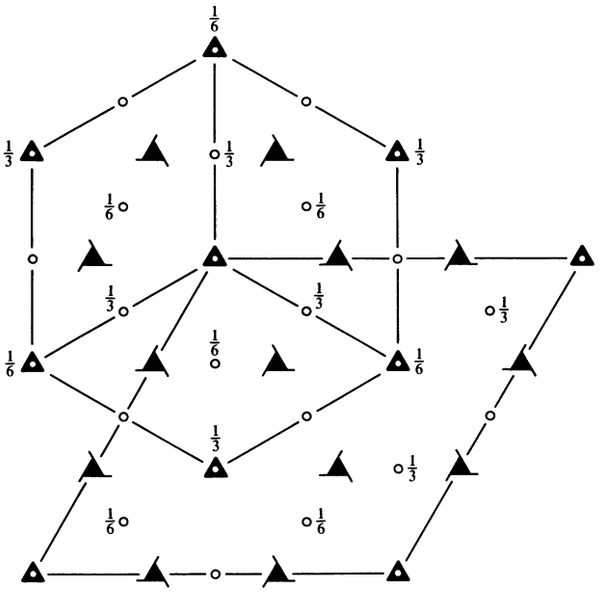
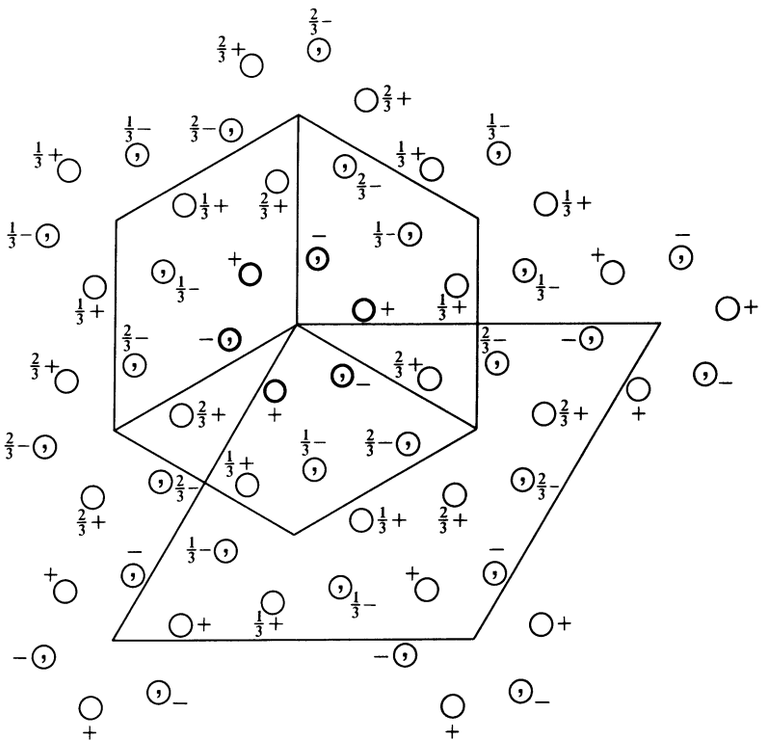
$R\bar{3}$ C_{3i}^{2} $\bar{3}$ Trigonal

No. 148 $R\bar{3}$ Patterson symmetry $R\bar{3}$

HEXAGONAL AXES





Origin at centre $(\bar{3})$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{6}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{6}$ $\frac{1}{2},0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ $0,\frac{1}{2},\frac{1}{6}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) $\bar{1}$ $0,0,0$ (5) $\bar{3}^+$ $0,0,z$; $0,0,0$ (6) $\bar{3}^-$ $0,0,z$; $0,0,0$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ (2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$ (3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$
(4) $\bar{1}$ $\frac{1}{3},\frac{1}{6},\frac{1}{6}$ (5) $\bar{3}^+$ $\frac{1}{3},-\frac{1}{3},z$; $\frac{1}{3},-\frac{1}{3},\frac{1}{6}$ (6) $\bar{3}^-$ $\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\frac{1}{6}$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ (2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$ (3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$
(4) $\bar{1}$ $\frac{1}{6},\frac{1}{3},\frac{1}{3}$ (5) $\bar{3}^+$ $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$ (6) $\bar{3}^-$ $-\frac{1}{3},\frac{1}{3},z$; $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
18	f	1	(1) x,y,z (4) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,\bar{z}$
9	e	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$
9	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$
6	c	3 .	$0,0,z$	$0,0,\bar{z}$	
3	b	$\bar{3}$.	$0,0,\frac{1}{2}$		
3	a	$\bar{3}$.	$0,0,0$		

Reflection conditions

General:

$hkil$: $-h+k+l=3n$
$hki0$: $-h+k=3n$
$hh\overline{2h}l$: $l=3n$
$h\bar{h}0l$: $h+l=3n$
$000l$: $l=3n$
$h\bar{h}00$: $h=3n$

Special: no extra conditions

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

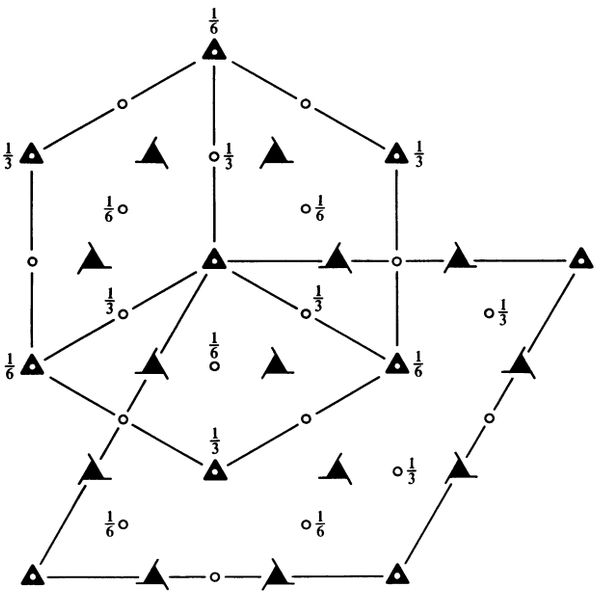
Along [100] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

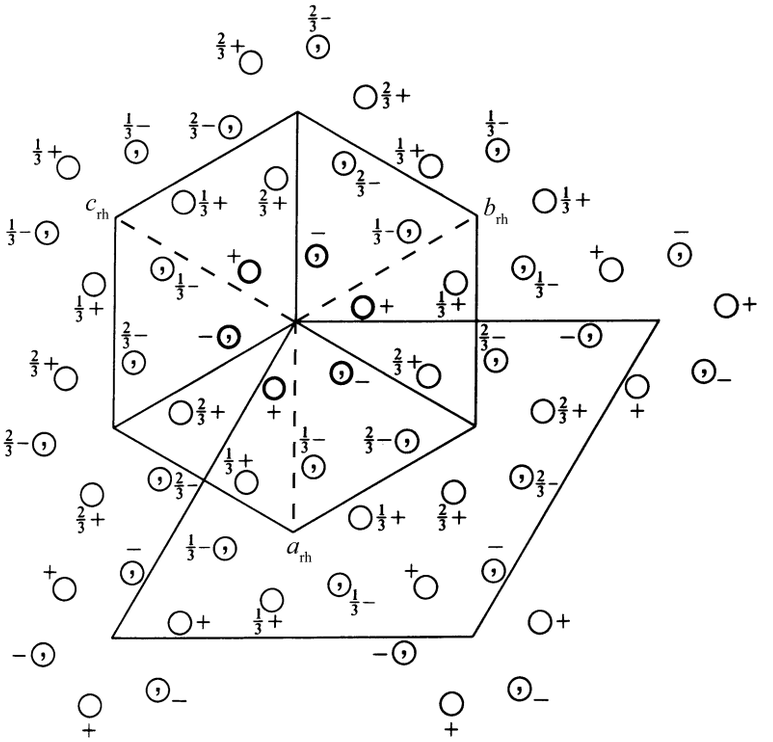
Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

No. 148 $R\bar{3}$

Patterson symmetry $R\bar{3}$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin at centre $(\bar{3})$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}; \quad z \le \min(x, y, 1-x, 1-y)$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ x,x,x (3) 3^- x,x,x
(4) $\bar{1}$ $0,0,0$ (5) $\bar{3}^+$ x,x,x; $0,0,0$ (6) $\bar{3}^-$ x,x,x; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	f	1	(1) x,y,z (4) $\bar{x},\bar{y},\bar{z}$	(2) z,x,y (5) $\bar{z},\bar{x},\bar{y}$	(3) y,z,x (6) $\bar{y},\bar{z},\bar{x}$	no conditions
						Special: no extra conditions
3	e	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	
3	d	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	
2	c	3 .	x,x,x	$\bar{x},\bar{x},\bar{x}$		
1	b	$\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
1	a	$\bar{3}$.	$0,0,0$			

Symmetry of special projections

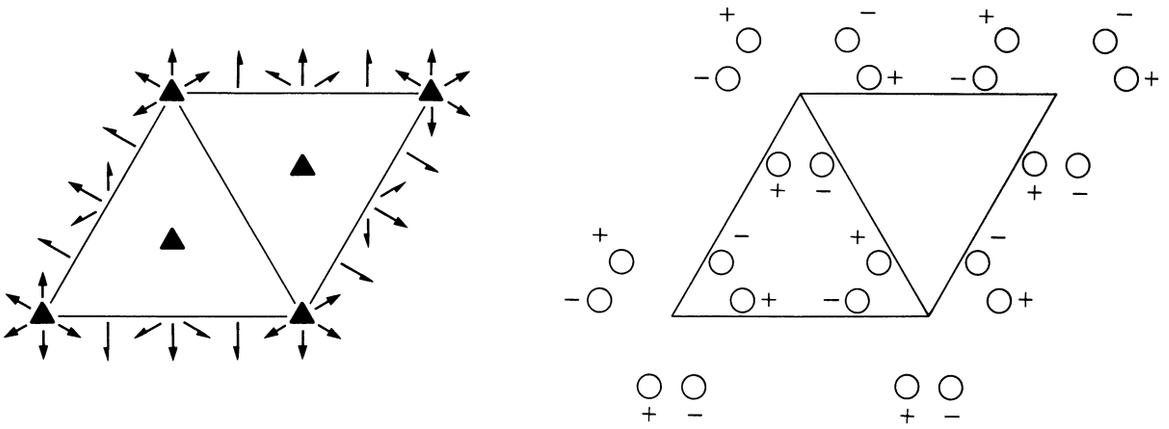
Along [111] $p6$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [1$\bar{1}$0] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along [2$\bar{1}\bar{1}$] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

$P312$ D_3^1 312 Trigonal

No. 149 $P312$ Patterson symmetry $P\bar{3}1m$



Origin at 312

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) 2 $x,\bar{x},0$ (5) 2 $x,2x,0$ (6) 2 $2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{y},\bar{x},\bar{z}$	(5) $\bar{x}+y,y,\bar{z}$	(6) $x,x-y,\bar{z}$	
						Special: no extra conditions
3	k	. . 2	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	j	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	
2	i	3 . .	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	h	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	g	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	f	3 . 2	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$			
1	e	3 . 2	$\frac{2}{3},\frac{1}{3},0$			
1	d	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			
1	c	3 . 2	$\frac{1}{3},\frac{2}{3},0$			
1	b	3 . 2	$0,0,\frac{1}{2}$			
1	a	3 . 2	$0,0,0$			

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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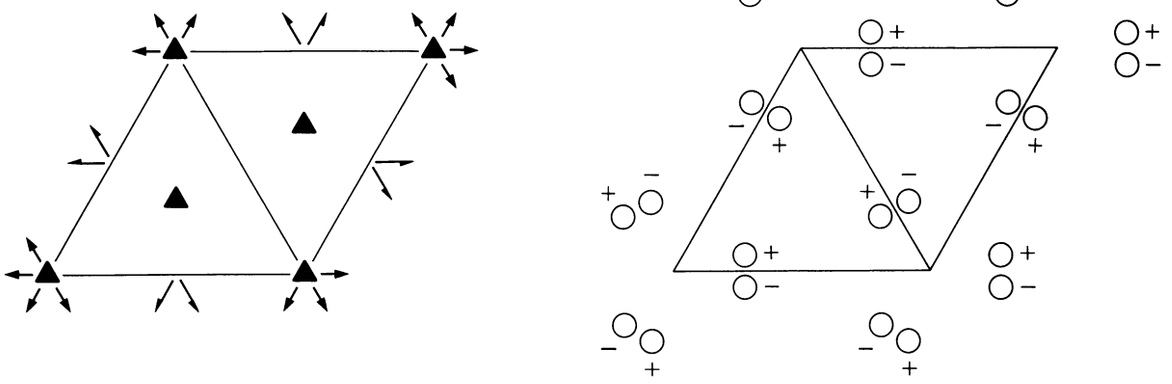
Trigonal 321 D_3^2 $P321$

Patterson symmetry $P\bar{3}m1$ $P321$ No. 150



Origin at 321

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) 2 $x,x,0$ (5) 2 $x,0,0$ (6) 2 $0,y,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$	
						Special: no extra conditions
3	f	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	e	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	
2	d	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	c	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	b	3 2 .	$0,0,\frac{1}{2}$			
1	a	3 2 .	$0,0,0$			

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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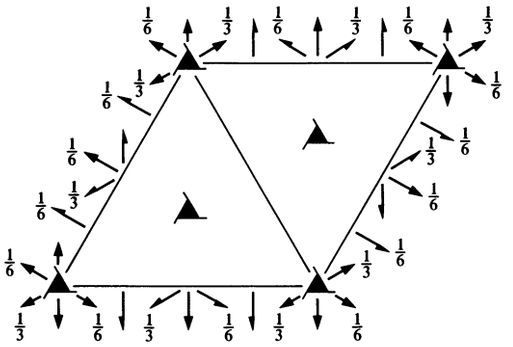
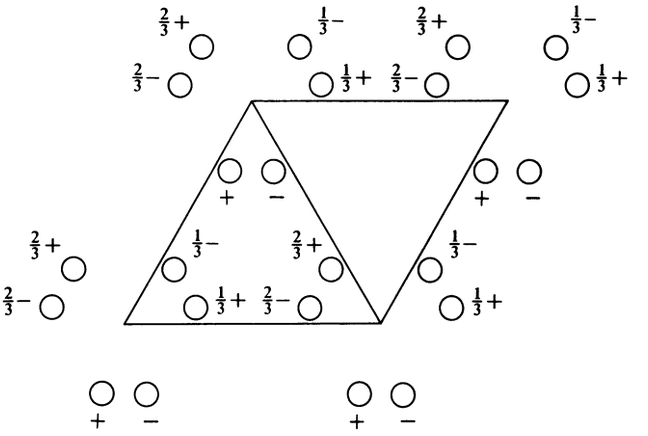
$P3_112$ D_3^3 312 Trigonal

No. 151 $P3_112$ Patterson symmetry $P\bar{3}1m$





Origin on $2[2\,1\,0]$ at $3_1\,1\,(1,1,2)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$

(4) 2 $x,\bar{x},\frac{1}{3}$ (5) 2 $x,2x,\frac{1}{6}$ (6) 2 $2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*c*	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l: l = 3n$
			(4) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(5) $\bar{x}+y,y,\bar{z}+\frac{1}{3}$	(6) $x,x-y,\bar{z}$	
						Special: no extra conditions
3	*b*	. . 2	$x,\bar{x},\frac{5}{6}$	$x,2x,\frac{1}{6}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	*a*	. . 2	$x,\bar{x},\frac{1}{3}$	$x,2x,\frac{2}{3}$	$2\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{6}$

Along [210] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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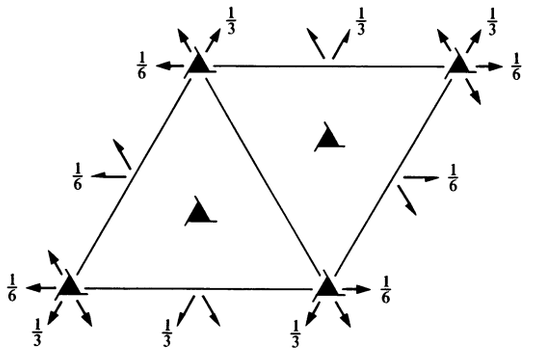
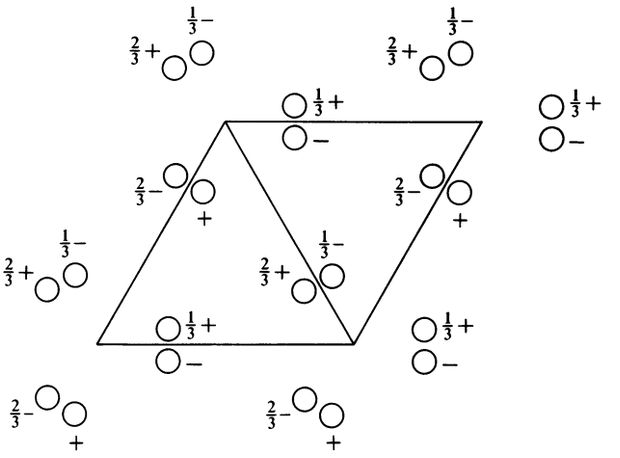
Trigonal 321 D_3^4 $P3_121$

Patterson symmetry $P\bar{3}m1$ $P3_121$ No. 152





Origin on $2[1\,1\,0]$ at $3_1\,(1,1,2)\,1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0\quad 0,1,0$

$0,0,\frac{1}{6}\quad 1,0,\frac{1}{6}\quad 1,1,\frac{1}{6}\quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$

(4) 2 $x,x,0$ (5) 2 $x,0,\frac{1}{3}$ (6) 2 $0,y,\frac{1}{6}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6	c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l: l = 3n$
		(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}+\frac{2}{3}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$	
					Special: no extra conditions
3	b . 2 .	$x,0,\frac{5}{6}$	$0,x,\frac{1}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	a . 2 .	$x,0,\frac{1}{3}$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{3}$

Along [210] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{6}$

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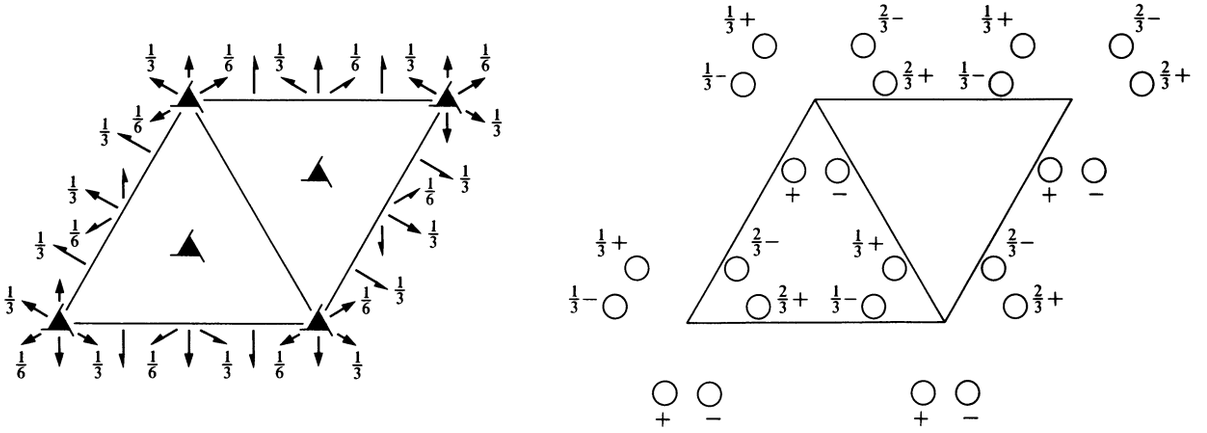
$P3_212$ D_3^5 312 Trigonal

No. 153 $P3_212$ Patterson symmetry $P\bar{3}1m$



Origin on $2[2\,1\,0]$ at $3_2\,1\,(1,1,2)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$

(4) 2 $x,\bar{x},\frac{1}{6}$ (5) 2 $x,2x,\frac{1}{3}$ (6) 2 $2x,x,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6	c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l: l = 3n$
		(4) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(5) $\bar{x}+y,y,\bar{z}+\frac{2}{3}$	(6) $x,x-y,\bar{z}$	
					Special: no extra conditions
3	b . . 2	$x,\bar{x},\frac{1}{6}$	$x,2x,\frac{5}{6}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	a . . 2	$x,\bar{x},\frac{2}{3}$	$x,2x,\frac{1}{3}$	$2\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}' = \mathbf{a} \quad \mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b}) \quad \mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{3}$

Along [210] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{b} \quad \mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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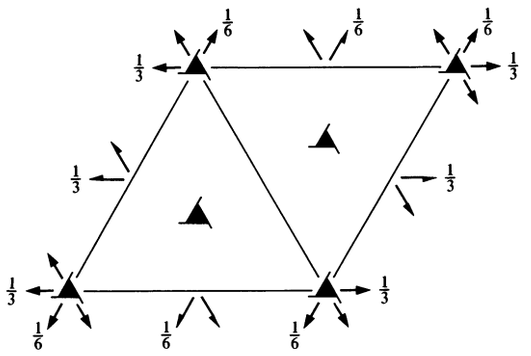
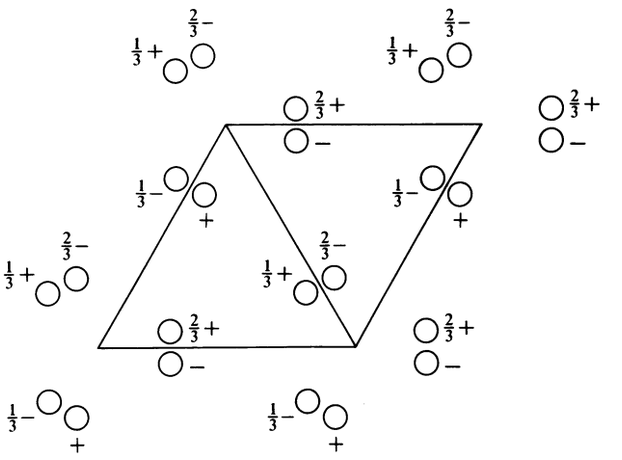
Trigonal 321 D_3^6 $P3_221$

Patterson symmetry $P\bar{3}m1$ $P3_221$ No. 154





Origin on $2[1\,1\,0]$ at $3_2\,(1,1,2)\,1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0\quad 0,1,0$

$0,0,\frac{1}{6}\quad 1,0,\frac{1}{6}\quad 1,1,\frac{1}{6}\quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$

(4) 2 $x,x,0$ (5) 2 $x,0,\frac{1}{6}$ (6) 2 $0,y,\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6	c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l: l = 3n$
		(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{3}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$	
					Special: no extra conditions
3	b . 2 .	$x,0,\frac{1}{6}$	$0,x,\frac{5}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	a . 2 .	$x,0,\frac{2}{3}$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},0$	

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,\frac{1}{6}$

Along [210] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{3}$

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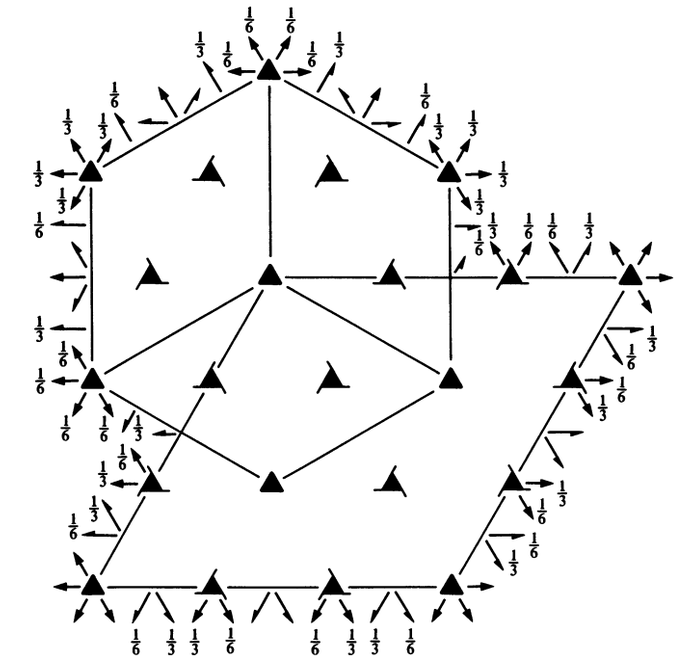
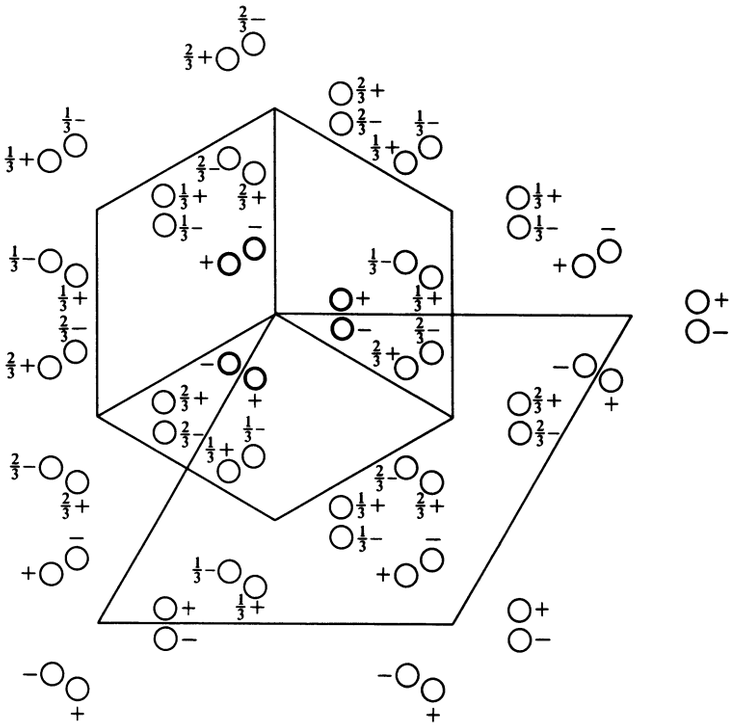
$R32$ D_3^7 32 Trigonal

No. 155 $R32$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin at 32

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{6}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{6}$ $\frac{1}{2},0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ $0,\frac{1}{2},\frac{1}{6}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $x,x,0$	(5) 2 $x,0,0$	(6) 2 $0,y,0$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$
(4) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{6},\frac{1}{6}$	(5) $2(\frac{1}{2},0,0)$ $x,\frac{1}{6},\frac{1}{6}$	(6) 2 $\frac{1}{3},y,\frac{1}{6}$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$
(4) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{6},\frac{1}{3}$	(5) 2 $x,\frac{1}{3},\frac{1}{3}$	(6) $2(0,\frac{1}{2},0)$ $\frac{1}{6},y,\frac{1}{3}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	Reflection conditions
18	f	1	(1) x,y,z (4) $y,x,\bar{z}$	(2) $\bar{y},x-y,z$ (5) $x-y,\bar{y},\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x},\bar{x}+y,\bar{z}$	General: $hkil$: $-h+k+l=3n$ $hki0$: $-h+k=3n$ $hh\overline{2h}l$: $l=3n$ $h\bar{h}0l$: $h+l=3n$ $000l$: $l=3n$ $h\bar{h}00$: $h=3n$ Special: no extra conditions
9	e	. 2	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
9	d	. 2	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	
6	c	3 .	$0,0,z$	$0,0,\bar{z}$		
3	b	3 2	$0,0,\frac{1}{2}$			
3	a	3 2	$0,0,0$			

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

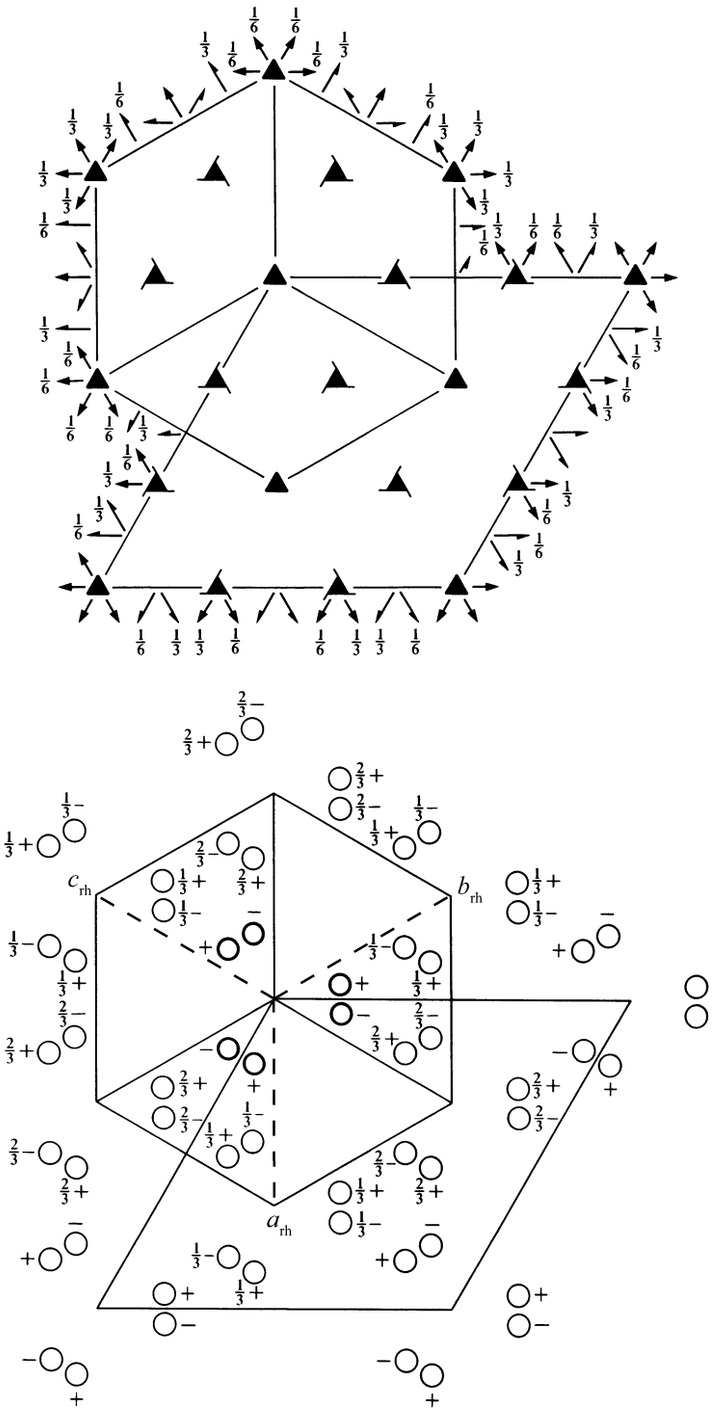
Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

No. 155 $R32$

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin at 32

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}; \quad z \le \min(x, y, 1-x, 1-y)$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ x,x,x (3) 3^- x,x,x
(4) 2 $\bar{x},0,x$ (5) 2 $x,\bar{x},0$ (6) 2 $0,y,\bar{y}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*f*	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
			(4) $\bar{z},\bar{y},\bar{x}$	(5) $\bar{y},\bar{x},\bar{z}$	(6) $\bar{x},\bar{z},\bar{y}$	
						Special: no extra conditions
3	*e*	. 2	$x,\bar{x},\frac{1}{2}$	$\frac{1}{2},x,\bar{x}$	$\bar{x},\frac{1}{2},x$	
3	*d*	. 2	$x,\bar{x},0$	$0,x,\bar{x}$	$\bar{x},0,x$	
2	*c*	3 .	x,x,x	$\bar{x},\bar{x},\bar{x}$		
1	*b*	3 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
1	*a*	3 2	$0,0,0$			

Symmetry of special projections

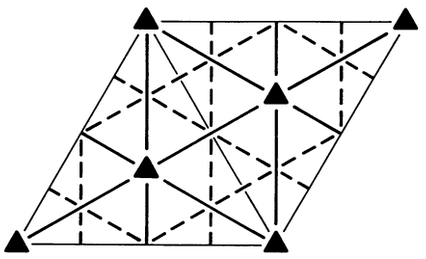
Along $[111]$ $p3m1$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

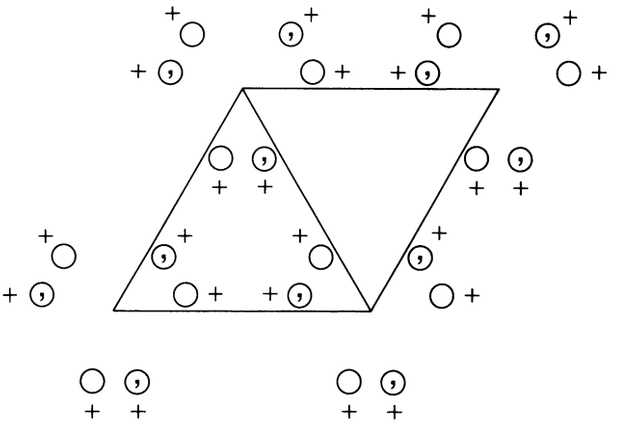
Along $[1\bar{1}0]$ $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

Along $[2\bar{1}\bar{1}]$ $p11m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

$P3m1$ C_{3v}^{1} $3m1$ Trigonal

No. 156 $P3m1$ Patterson symmetry $P\bar{3}m1$





Origin on $3m1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le 1$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$
$0,0,1$ $\frac{2}{3},\frac{1}{3},1$ $\frac{1}{3},\frac{2}{3},1$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) m $x,\bar{x},z$ (5) m $x,2x,z$ (6) m $2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	e	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$	
						Special: no extra conditions
3	d	$.m.$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	
1	c	$3m.$	$\frac{2}{3},\frac{1}{3},z$			
1	b	$3m.$	$\frac{1}{3},\frac{2}{3},z$			
1	a	$3m.$	$0,0,z$			

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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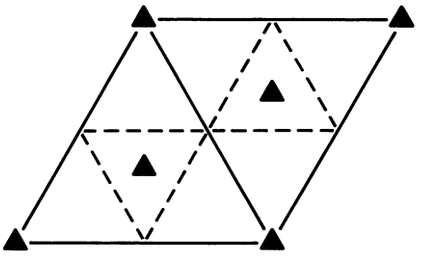
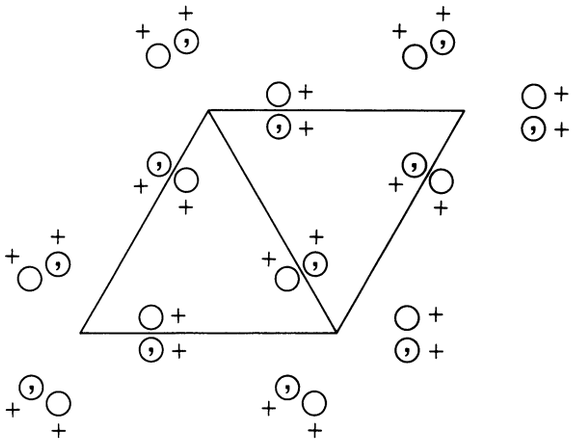
Trigonal $3\,1\,m$ C_{3v}^2 $P\,3\,1\,m$

Patterson symmetry $P\bar{3}\,1\,m$ $P\,3\,1\,m$ No. 157





Origin on $3\,1\,m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le (y+1)/2$; $y \le \min(1-x, x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$ $\frac{1}{2},\frac{1}{2},1$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) m x,x,z (5) m $x,0,z$ (6) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) y,x,z	(5) $x-y,\bar{y},z$	(6) $\bar{x},\bar{x}+y,z$	
						Special: no extra conditions
3	c	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	
2	b	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$		
1	a	$3.m$	$0,0,z$			

Symmetry of special projections

Along [001] $p\,3\,1\,m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x, \frac{1}{2}x, 0$

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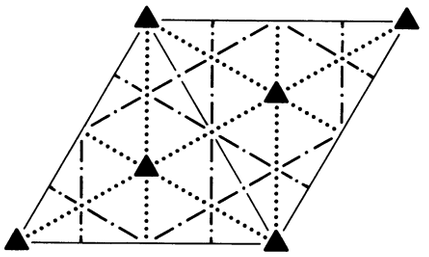
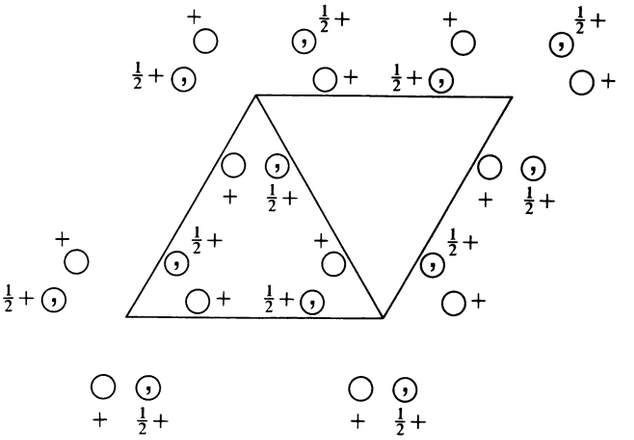
$P3c1$ C_{3v}^3 $3m1$ Trigonal

No. 158 $P3c1$ Patterson symmetry $P\bar{3}m1$





Origin on $3c1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) c $x,\bar{x},z$ (5) c $x,2x,z$ (6) c $2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	d	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$h\bar{h}0l$: $l=2n$
			(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$	$000l$: $l=2n$
						Special: as above, plus
2	c	$3..$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$		$hkil$: $l=2n$
2	b	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$		$hkil$: $l=2n$
2	a	$3..$	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p3m1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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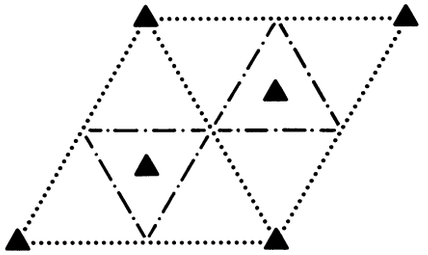
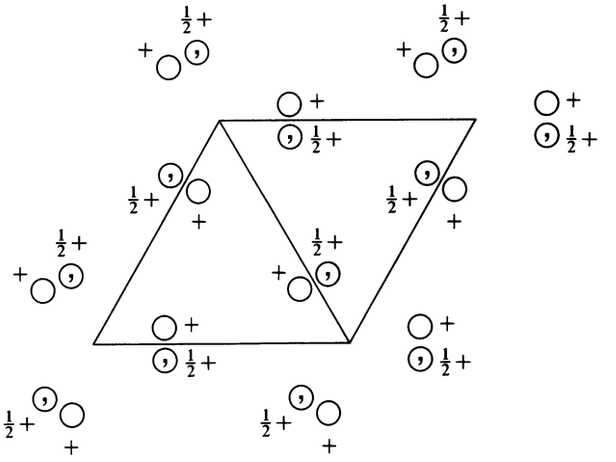
Trigonal $31m$ C_{3v}^4 $P31c$

Patterson symmetry $P\bar{3}1m$ $P31c$ No. 159





Origin on $31c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) c x,x,z (5) c $x,0,z$ (6) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 c 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hh\overline{2h}l$: $l=2n$
	(4) $y,x,z+\frac{1}{2}$	(5) $x-y,\bar{y},z+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,z+\frac{1}{2}$	$000l$: $l=2n$
				Special: as above, plus
2 b 3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$		$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2 a 3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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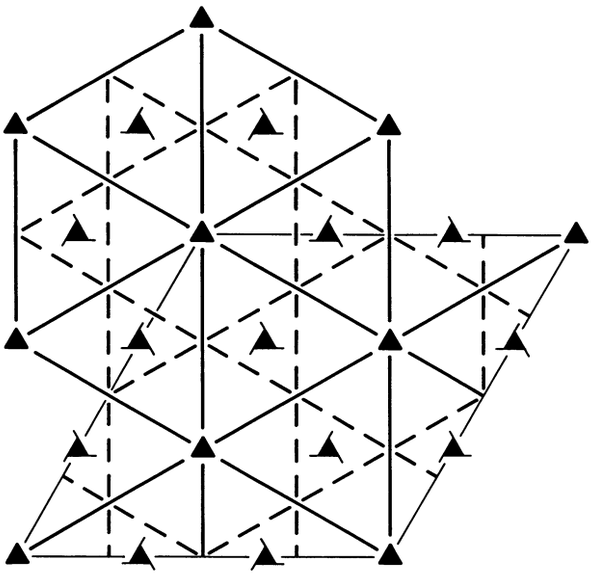
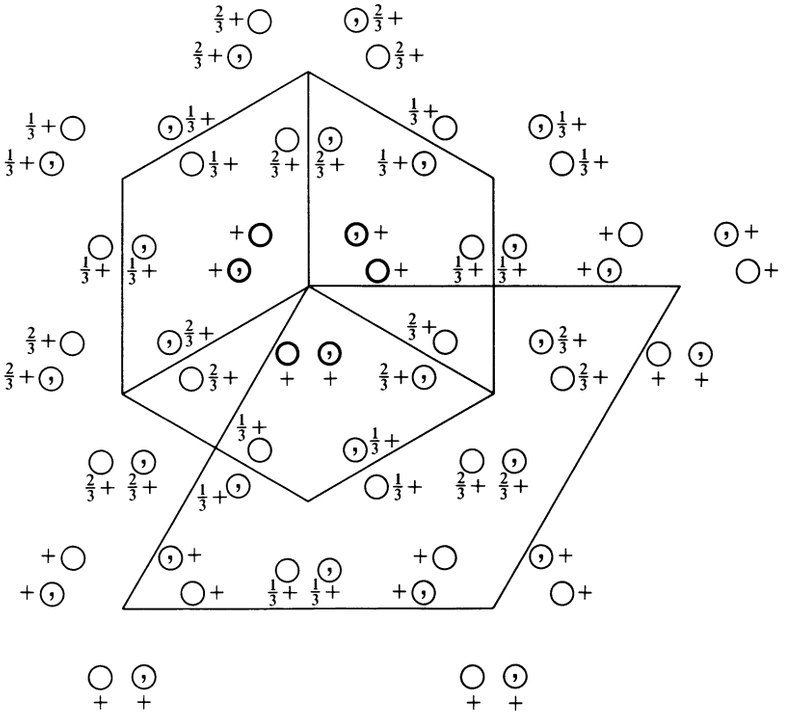
$R3m$ C_{3v}^5 $3m$ Trigonal

No. 160 $R3m$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin on $3m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{3}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$
$0,0,\frac{1}{3}$ $\frac{2}{3},\frac{1}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3},\frac{1}{3}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) m $x,\bar{x},z$	(5) m $x,2x,z$	(6) m $2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$
(4) $g(\frac{1}{6},-\frac{1}{6},\frac{1}{3})$ $x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{6},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{4},2x,z$	(6) $g(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ $2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$
(4) $g(-\frac{1}{6},\frac{1}{6},\frac{2}{3})$ $x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ $x,2x,z$	(6) $g(\frac{1}{3},\frac{1}{6},\frac{2}{3})$ $2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$		Reflection conditions
18	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$
					General:
					$hkil$: $-h+k+l=3n$
					$hki0$: $-h+k=3n$
					$hh\overline{2h}l$: $l=3n$
					$h\bar{h}0l$: $h+l=3n$
					$000l$: $l=3n$
					$h\bar{h}00$: $h=3n$
					Special: no extra conditions
9	b	. m	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$
3	a	3 m	$0,0,z$		

Symmetry of special projections

Along [001] $p3\,1m$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

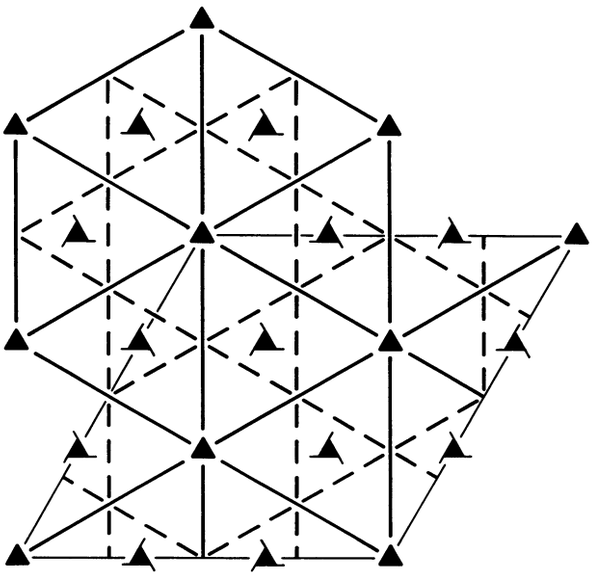
Along [100] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

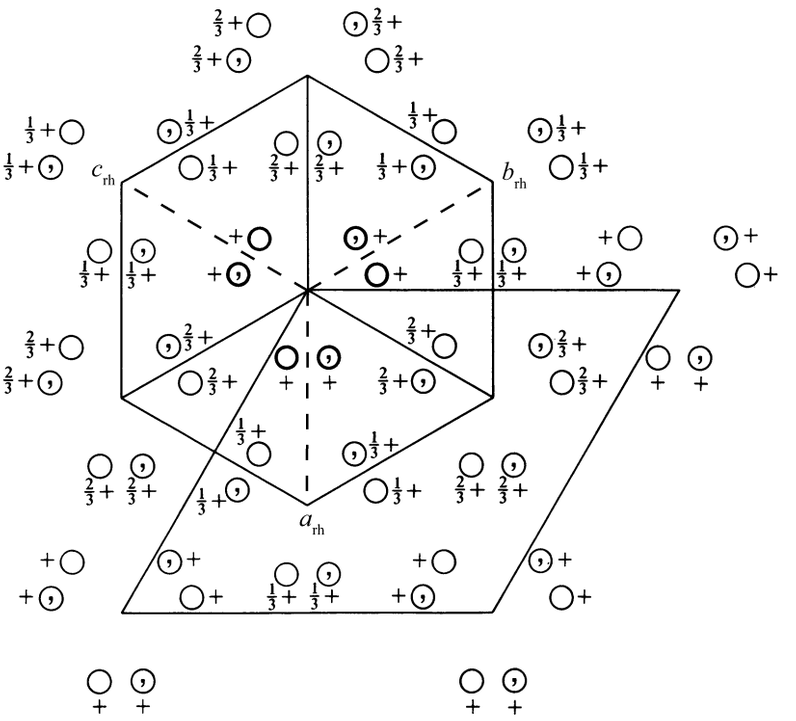
Along [210] $p\,1\,m\,1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

No. 160 $R3m$

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin on $3m$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le 1;\quad y \le x;\quad z \le y$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0\quad 1,1,1$

Symmetry operations

(1) 1 (2) 3^+ x,x,x (3) 3^- x,x,x
(4) m x,y,x (5) m x,x,z (6) m x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 c 1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
	(4) z,y,x	(5) y,x,z	(6) x,z,y	
				Special: no extra conditions
3 b $.m$	x,y,x	x,x,y	y,x,x	
1 a $3m$	x,x,x			

Symmetry of special projections

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

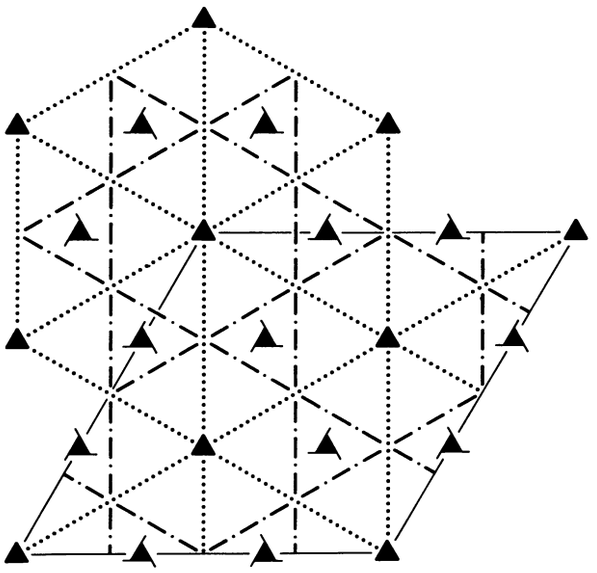
Along [1$\bar{1}$0] $p1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

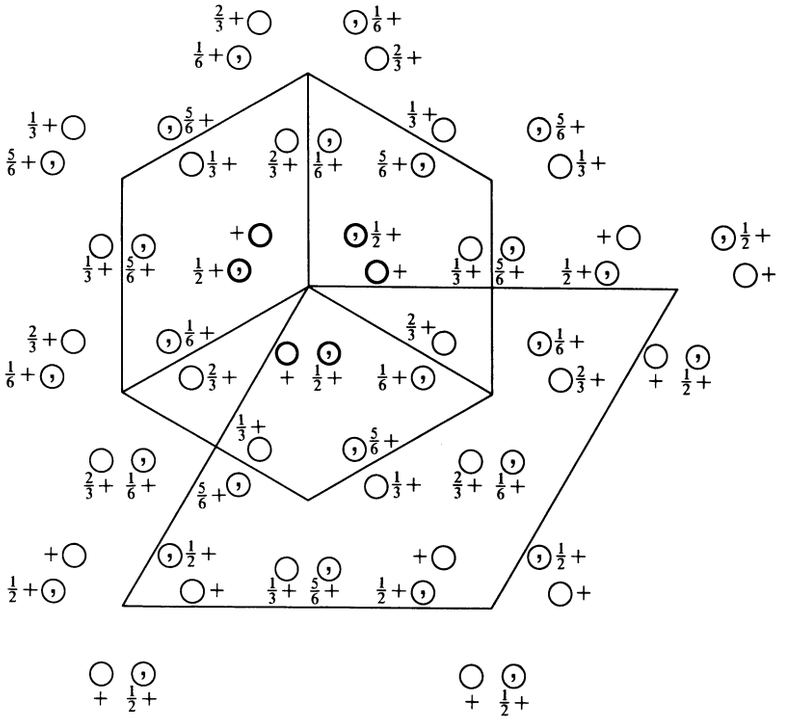
Along [2$\bar{1}\bar{1}$] $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

$R3c$ C_{3v}^{6} $3m$ Trigonal

No. 161 $R3c$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin on $3c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{6}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{6}$ $\frac{1}{2},0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$ $0,\frac{1}{2},\frac{1}{6}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) c $x,\bar{x},z$	(5) c $x,2x,z$	(6) c $2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$
(4) $g(\frac{1}{6},-\frac{1}{6},\frac{5}{6})$ $x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{6},\frac{1}{3},\frac{5}{6})$ $x+\frac{1}{4},2x,z$	(6) $g(\frac{2}{3},\frac{1}{3},\frac{5}{6})$ $2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$
(4) $g(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{2},\bar{x},z$	(5) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})$ $x,2x,z$	(6) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ $2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$ $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$			Reflection conditions
				General:
18 b 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$
	(4) $\bar{y},\bar{x},z+\frac{1}{2}$	(5) $\bar{x}+y,y,z+\frac{1}{2}$	(6) $x,x-y,z+\frac{1}{2}$	$hki0$: $-h+k=3n$
				$hh\overline{2h}l$: $l=3n$
				$h\bar{h}0l$: $h+l=3n$, $l=2n$
				$000l$: $l=6n$
				$h\bar{h}00$: $h=3n$
				Special: as above, plus
6 a 3 .	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

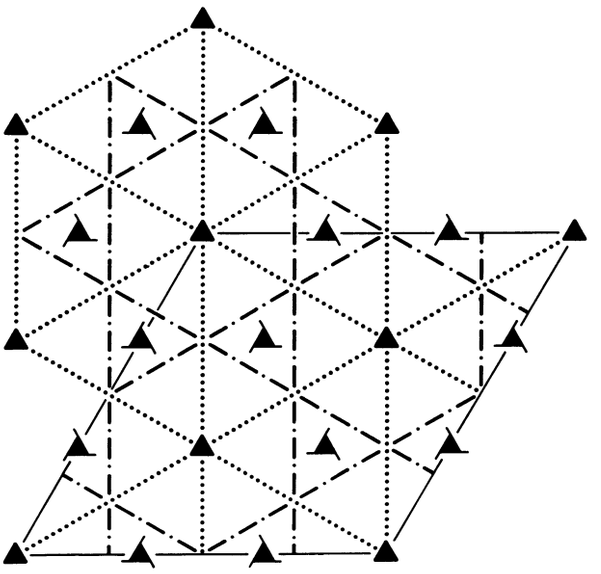
Along [100] $p1$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}+4\mathbf{b}+\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

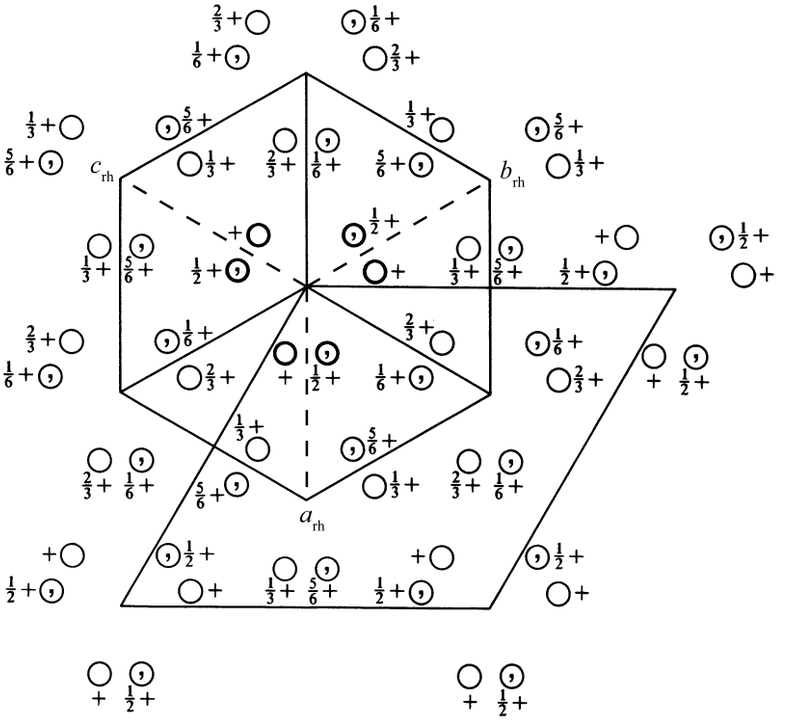
Along [210] $p1g1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

No. 161 $R3c$

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES





Heights refer to hexagonal axes

Origin on $3c$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le 1;\quad y \le x;\quad z \le y$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0\quad 1,1,1$

Symmetry operations

(1) 1 (2) 3^+ x,x,x (3) 3^- x,x,x
(4) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x (5) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z (6) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 b 1	(1) x,y,z	(2) z,x,y	(3) y,z,x	hhl: $l=2n$
	(4) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(5) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(6) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	hhh: $h=2n$
				Special: as above, plus
2 a 3.	x,x,x	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$		hkl: $h+k+l=2n$

Symmetry of special projections

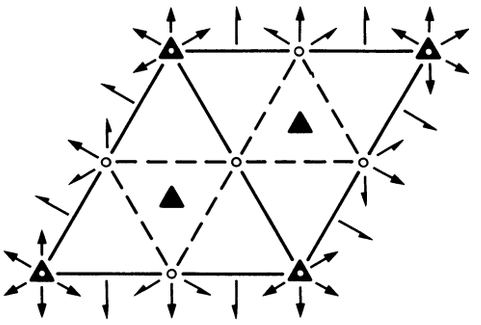
Along [111] $p3\,1m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

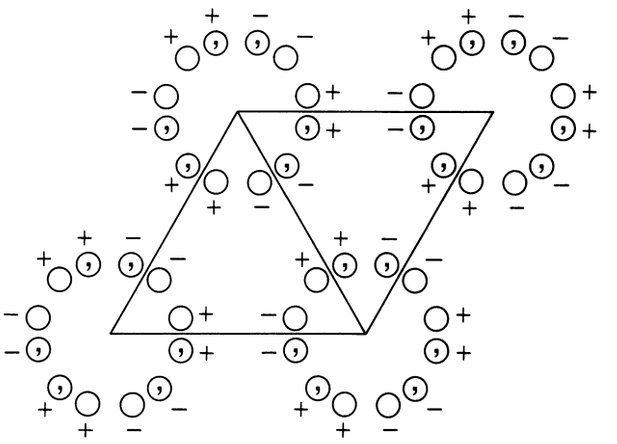
Along [1$\bar{1}$0] $p\,1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\bar{x},0$

Along [2$\bar{1}\bar{1}$] $p\,1\,g\,1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

$P\bar{3}1m$ D_{3d}^{1} $\bar{3}1m$ Trigonal

No. 162 $P\bar{3}12/m$ Patterson symmetry $P\bar{3}1m$





Origin at centre $(\bar{3}1m)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) 2 $x,\bar{x},0$
(5) 2 $x,2x,0$
(6) 2 $2x,x,0$
(7) $\bar{1}$ $0,0,0$
(8) $\bar{3}^+$ $0,0,z$; $0,0,0$
(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) m x,x,z
(11) m $x,0,z$
(12) m $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $\bar{y},\bar{x},\bar{z}$	(5) $\bar{x}+y,y,\bar{z}$	(6) $x,x-y,\bar{z}$				
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$				
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$				
									Special: no extra conditions
6	k	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$	
6	j	$..2$	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	
6	i	$..2$	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$	$\bar{x},2\bar{x},0$	$2x,x,0$	
4	h	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z$			
3	g	$..2/m$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	f	$..2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	e	$3.m$	$0,0,z$	$0,0,\bar{z}$					
2	d	3.2	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	3.2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	$\bar{3}.m$	$0,0,\frac{1}{2}$						
1	a	$\bar{3}.m$	$0,0,0$						

Symmetry of special projections

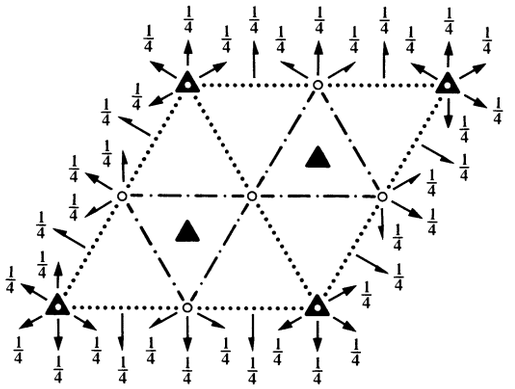
Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

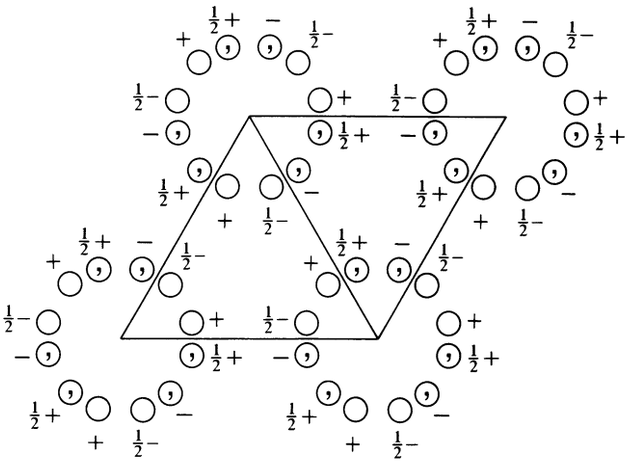
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P\bar{3}1c$ D_{3d}^2 $\bar{3}1m$ Trigonal

No. 163 $P\bar{3}12/c$ Patterson symmetry $P\bar{3}1m$





Origin at centre $(\bar{3})$ at $\bar{3}1c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) 2 $x,\bar{x},\frac{1}{4}$
(5) 2 $x,2x,\frac{1}{4}$
(6) 2 $2x,x,\frac{1}{4}$
(7) $\bar{1}$ $0,0,0$
(8) $\bar{3}^+$ $0,0,z$; $0,0,0$
(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) c x,x,z
(11) c $x,0,z$
(12) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z (4) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $y,x,z+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $x-y,\bar{y},z+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x,x-y,\bar{z}+\frac{1}{2}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				$hh\overline{2h}l$: $l=2n$ $000l$: $l=2n$
									Special: as above, plus
6	h	. . 2	$x,\bar{x},\frac{1}{4}$	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},x,\frac{3}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	no extra conditions
6	g	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	f	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	3 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
2	d	3 . 2	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	b	$\bar{3}$ . .	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	3 . 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

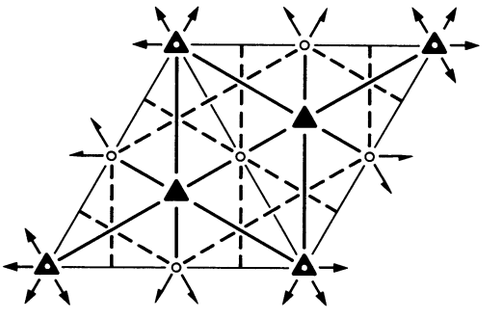
Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

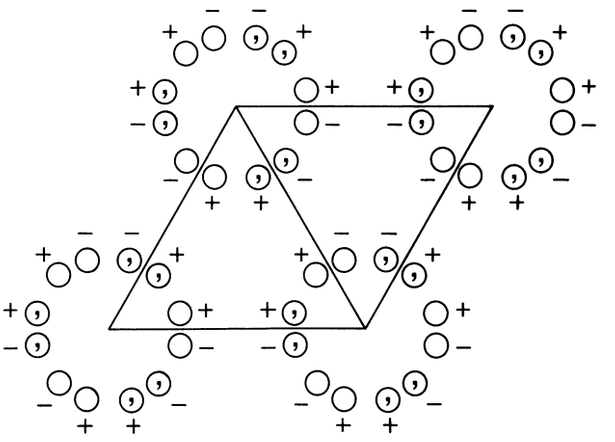
Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P\bar{3}m1$ D_{3d}^3 $\bar{3}m1$ Trigonal

No. 164 $P\bar{3}2/m1$ Patterson symmetry $P\bar{3}m1$





Origin at centre $(\bar{3}m1)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$
$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $x,x,0$	(5) 2 $x,0,0$	(6) 2 $0,y,0$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ $0,0,z$; $0,0,0$	(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) m $x,\bar{x},z$	(11) m $x,2x,z$	(12) m $2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
12 j 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
	(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$	
	(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	
	(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$	
				Special: no extra conditions
6 i . m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$ $2x,x,\bar{z}$ $\bar{x},2\bar{x},\bar{z}$
6 h . 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $x,x,\frac{1}{2}$
6 g . 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$ $0,\bar{x},0$ $x,x,0$
3 f . $2/m$.	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
3 e . $2/m$.	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
2 d $3m$.	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2 c $3m$.	$0,0,z$	$0,0,\bar{z}$		
1 b $\bar{3}m$.	$0,0,\frac{1}{2}$			
1 a $\bar{3}m$.	$0,0,0$			

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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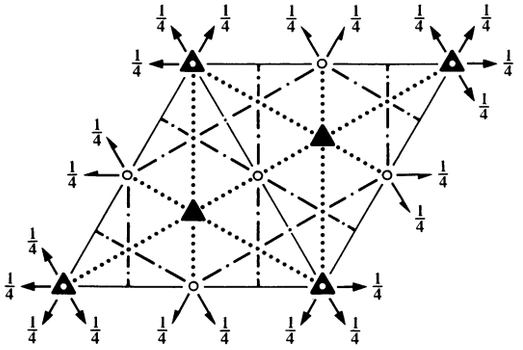
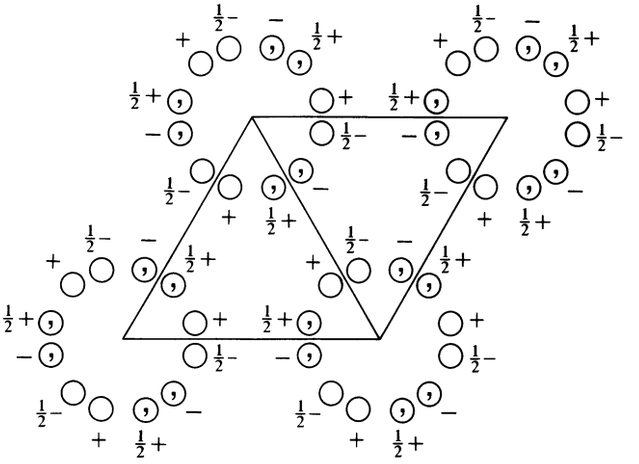
Trigonal $\bar{3}m1$ D_{3d}^4 $P\bar{3}c1$

Patterson symmetry $P\bar{3}m1$ $P\bar{3}2/c1$ No. 165





Origin at centre $(\bar{3})$ at $\bar{3}c1$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $x,x,\frac{1}{4}$	(5) 2 $x,0,\frac{1}{4}$	(6) 2 $0,y,\frac{1}{4}$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ $0,0,z$; $0,0,0$	(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) c $x,\bar{x},z$	(11) c $x,2x,z$	(12) c $2x,x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	g	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$h\bar{h}0l$: $l=2n$
			(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$				$000l$: $l=2n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$				
			(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$				
									Special: as above, plus
6	f	.2.	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	no extra conditions
6	e	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	d	3..	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$			$hkil$: $l=2n$
4	c	3..	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
2	b	$\bar{3}$..	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	32.	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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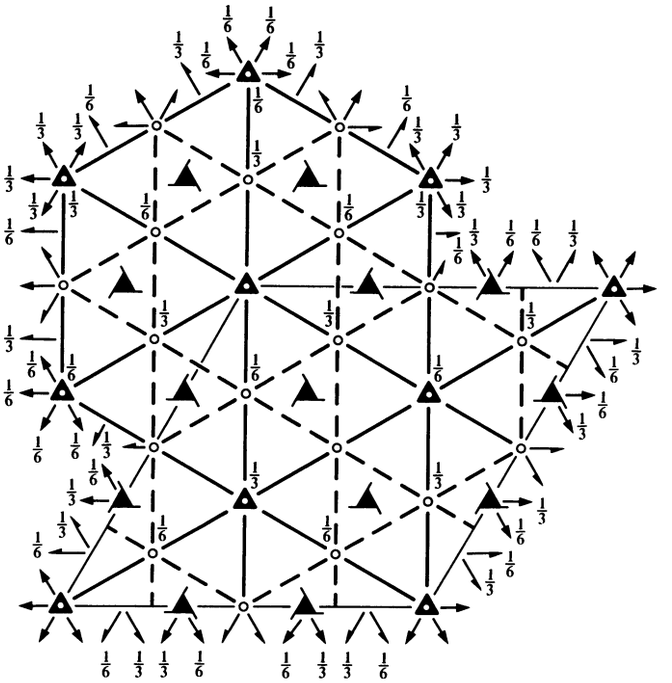
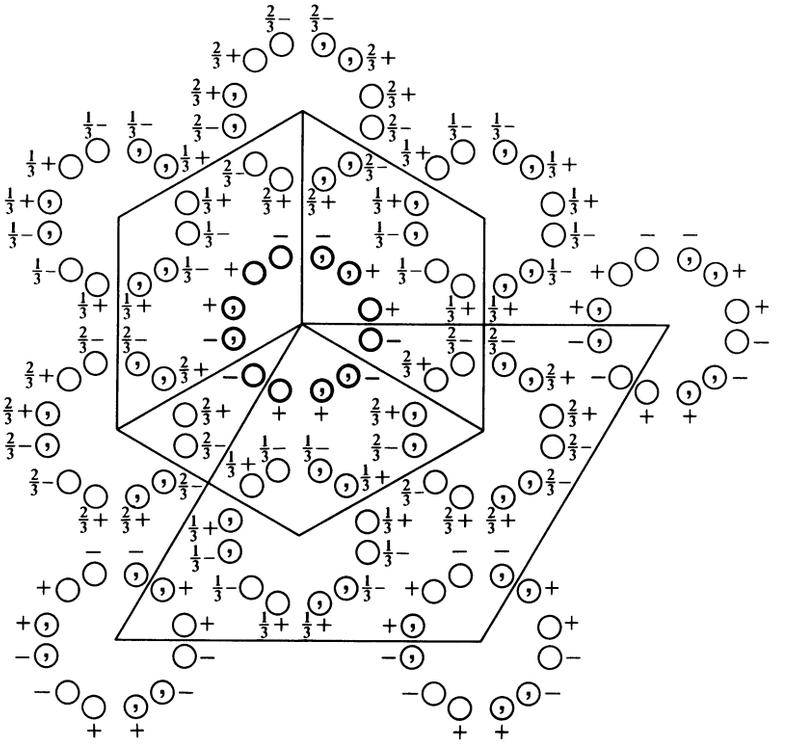
$R\bar{3}m$ D_{3d}^5 $\bar{3}m$ Trigonal

No. 166 $R\bar{3}2/m$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin at centre $(\bar{3}m)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{6}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$

$0,0,\frac{1}{6}$ $\frac{2}{3},\frac{1}{3},\frac{1}{6}$ $\frac{1}{3},\frac{2}{3},\frac{1}{6}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $x,x,0$	(5) 2 $x,0,0$	(6) 2 $0,y,0$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ $0,0,z$; $0,0,0$	(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) m $x,\bar{x},z$	(11) m $x,2x,z$	(12) m $2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$
(4) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{6},\frac{1}{6}$	(5) $2(\frac{1}{2},0,0)$ $x,\frac{1}{6},\frac{1}{6}$	(6) 2 $\frac{1}{3},y,\frac{1}{6}$
(7) $\bar{1}$ $\frac{1}{3},\frac{1}{6},\frac{1}{6}$	(8) $\bar{3}^+$ $\frac{1}{3},-\frac{1}{3},z$; $\frac{1}{3},-\frac{1}{3},\frac{1}{6}$	(9) $\bar{3}^-$ $\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\frac{1}{6}$
(10) $g(\frac{1}{6},-\frac{1}{6},\frac{1}{3})$ $x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{6},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{4},2x,z$	(12) $g(\frac{2}{3},\frac{1}{3},\frac{1}{3})$ $2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$
(4) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{6},\frac{1}{3}$	(5) 2 $x,\frac{1}{3},\frac{1}{3}$	(6) $2(0,\frac{1}{2},0)$ $\frac{1}{6},y,\frac{1}{3}$
(7) $\bar{1}$ $\frac{1}{6},\frac{1}{3},\frac{1}{3}$	(8) $\bar{3}^+$ $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$	(9) $\bar{3}^-$ $-\frac{1}{3},\frac{1}{3},z$; $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$
(10) $g(-\frac{1}{6},\frac{1}{6},\frac{2}{3})$ $x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{3},\frac{2}{3},\frac{2}{3})$ $x,2x,z$	(12) $g(\frac{1}{3},\frac{1}{6},\frac{2}{3})$ $2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	Reflection conditions
36	i	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	General:
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$	$hkil$: $-h+k+l=3n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	$hki0$: $-h+k=3n$
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$	$h\bar{h}2\bar{h}l$: $l=3n$
						$h\bar{h}0l$: $h+l=3n$
						$000l$: $l=3n$
						$h\bar{h}00$: $h=3n$
						Special: no extra conditions
18	h	. m	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$ $2x,x,\bar{z}$ $\bar{x},2\bar{x},\bar{z}$
18	g	. 2	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $x,x,\frac{1}{2}$
18	f	. 2	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$ $0,\bar{x},0$ $x,x,0$
9	e	. $2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	
9	d	. $2/m$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
6	c	3 m	$0,0,z$	$0,0,\bar{z}$		
3	b	$\bar{3}$ m	$0,0,\frac{1}{2}$			
3	a	$\bar{3}$ m	$0,0,0$			

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

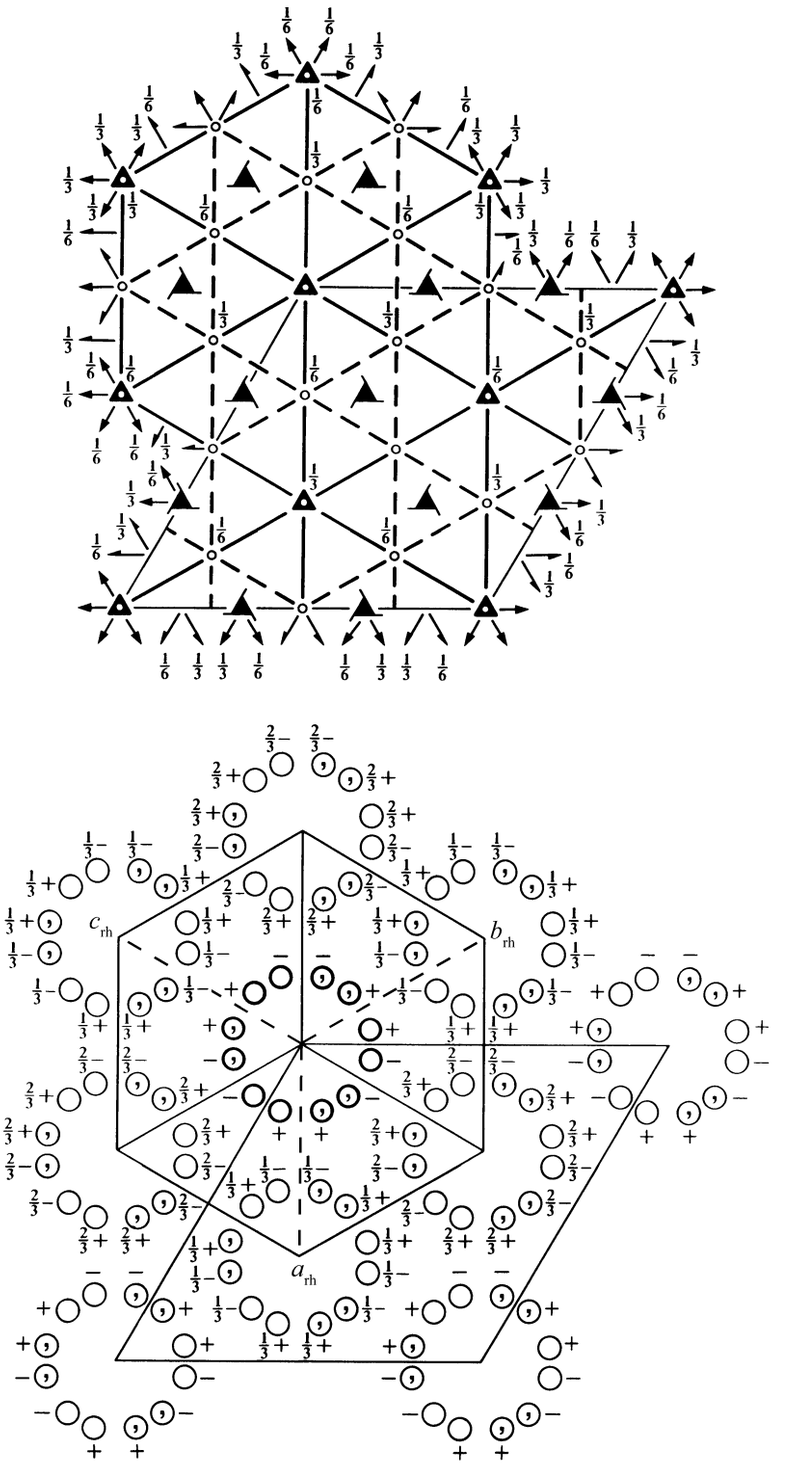
Along [100] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

No. 166 $R\bar{3}2/m$

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin at centre $(\bar{3}m)$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{2}; \quad y \le x; \quad z \le \min(y, 1-x)$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) 2 $\bar{x},0,x$	(5) 2 $x,\bar{x},0$	(6) 2 $0,y,\bar{y}$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ x,x,x; $0,0,0$	(9) $\bar{3}^-$ x,x,x; $0,0,0$
(10) m x,y,x	(11) m x,x,z	(12) m x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	i	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	no conditions
			(4) $\bar{z},\bar{y},\bar{x}$	(5) $\bar{y},\bar{x},\bar{z}$	(6) $\bar{x},\bar{z},\bar{y}$	
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$	
			(10) z,y,x	(11) y,x,z	(12) x,z,y	
						Special: no extra conditions
6	h	$.m$	x,y,x	x,x,y	y,x,x	$\bar{x},\bar{y},\bar{x}$ $\bar{y},\bar{x},\bar{x}$ $\bar{x},\bar{x},\bar{y}$
6	g	$.2$	$x,\bar{x},\frac{1}{2}$	$\frac{1}{2},x,\bar{x}$	$\bar{x},\frac{1}{2},x$	$\bar{x},x,\frac{1}{2}$ $\frac{1}{2},\bar{x},x$ $x,\frac{1}{2},\bar{x}$
6	f	$.2$	$x,\bar{x},0$	$0,x,\bar{x}$	$\bar{x},0,x$	$\bar{x},x,0$ $0,\bar{x},x$ $x,0,\bar{x}$
3	e	$.2/m$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	
3	d	$.2/m$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	
2	c	$3\,m$	x,x,x	$\bar{x},\bar{x},\bar{x}$		
1	b	$\bar{3}\,m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
1	a	$\bar{3}\,m$	$0,0,0$			

Symmetry of special projections

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

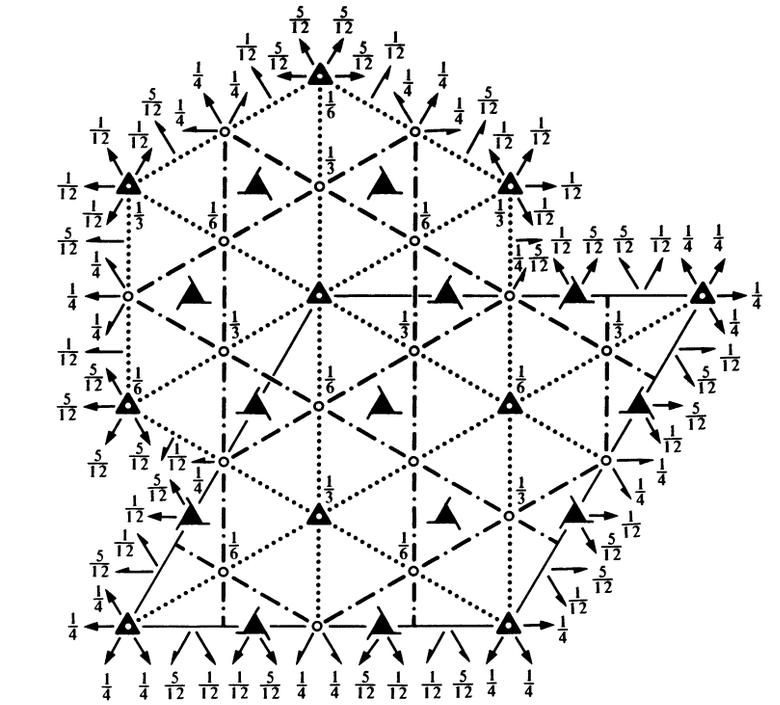
Along [1$\bar{1}$0] $p2$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\bar{x},0$

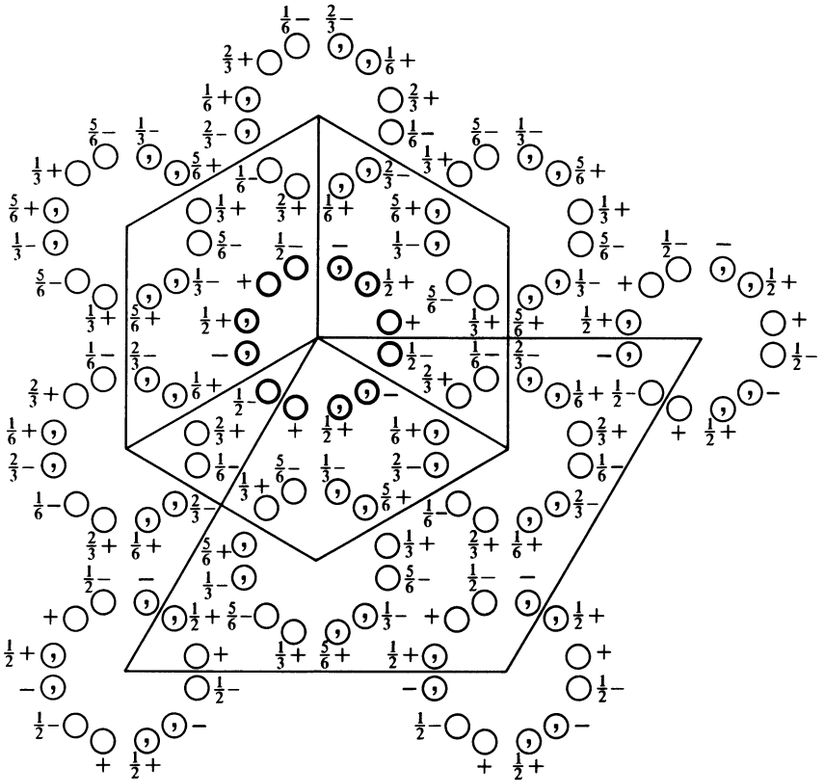
Along [2$\bar{1}\bar{1}$] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

$R\bar{3}c$ D_{3d}^6 $\bar{3}m$ Trigonal

No. 167 $R\bar{3}2/c$ Patterson symmetry $R\bar{3}m$

HEXAGONAL AXES





Origin at centre $(\bar{3})$ at $\bar{3}c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{12}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$

$0,0,\frac{1}{12}$ $\frac{1}{2},0,\frac{1}{12}$ $\frac{2}{3},\frac{1}{3},\frac{1}{12}$ $\frac{1}{3},\frac{2}{3},\frac{1}{12}$ $0,\frac{1}{2},\frac{1}{12}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $x,x,\frac{1}{4}$	(5) 2 $x,0,\frac{1}{4}$	(6) 2 $0,y,\frac{1}{4}$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ $0,0,z$; $0,0,0$	(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) c $x,\bar{x},z$	(11) c $x,2x,z$	(12) c $2x,x,z$

For $(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$ set

(1) $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$	(2) $3^+(0,0,\frac{1}{3})$ $\frac{1}{3},\frac{1}{3},z$	(3) $3^-(0,0,\frac{1}{3})$ $\frac{1}{3},0,z$
(4) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{6},\frac{5}{12}$	(5) $2(\frac{1}{2},0,0)$ $x,\frac{1}{6},\frac{5}{12}$	(6) 2 $\frac{1}{3},y,\frac{5}{12}$
(7) $\bar{1}$ $\frac{1}{3},\frac{1}{6},\frac{1}{6}$	(8) $\bar{3}^+$ $\frac{1}{3},-\frac{1}{3},z$; $\frac{1}{3},-\frac{1}{3},\frac{1}{6}$	(9) $\bar{3}^-$ $\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\frac{1}{6}$
(10) $g(\frac{1}{6},-\frac{1}{6},\frac{5}{6})$ $x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{6},\frac{1}{3},\frac{5}{6})$ $x+\frac{1}{4},2x,z$	(12) $g(\frac{2}{3},\frac{1}{3},\frac{5}{6})$ $2x,x,z$

For $(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$ set

(1) $t(\frac{1}{3},\frac{2}{3},\frac{2}{3})$	(2) $3^+(0,0,\frac{2}{3})$ $0,\frac{1}{3},z$	(3) $3^-(0,0,\frac{2}{3})$ $\frac{1}{3},\frac{1}{3},z$
(4) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{6},\frac{1}{12}$	(5) 2 $x,\frac{1}{3},\frac{1}{12}$	(6) $2(0,\frac{1}{2},0)$ $\frac{1}{6},y,\frac{1}{12}$
(7) $\bar{1}$ $\frac{1}{6},\frac{1}{3},\frac{1}{3}$	(8) $\bar{3}^+$ $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$	(9) $\bar{3}^-$ $-\frac{1}{3},\frac{1}{3},z$; $-\frac{1}{3},\frac{1}{3},\frac{1}{3}$
(10) $g(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{2},\bar{x},z$	(11) $g(\frac{1}{3},\frac{2}{3},\frac{1}{6})$ $x,2x,z$	(12) $g(\frac{1}{3},\frac{1}{6},\frac{1}{6})$ $2x-\frac{1}{2},x,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{2}{3},\frac{1}{3},\frac{1}{3})$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$	Reflection conditions
				General:
36 f 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$hkil$: $-h+k+l=3n$
	(4) $y,x,\bar{z}+\frac{1}{2}$	(5) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(6) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$	$hki\bar{0}$: $-h+k=3n$
	(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	$h\bar{h}2\bar{h}l$: $l=3n$
	(10) $\bar{y},\bar{x},z+\frac{1}{2}$	(11) $\bar{x}+y,y,z+\frac{1}{2}$	(12) $x,x-y,z+\frac{1}{2}$	$h\bar{h}0l$: $h+l=3n$, $l=2n$
				$000l$: $l=6n$
				$h\bar{h}00$: $h=3n$
				Special: as above, plus
18 e . 2	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$ $0,\bar{x},\frac{3}{4}$ $x,x,\frac{3}{4}$	no extra conditions
18 d $\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
12 c 3 .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	$hkil$: $l=2n$
6 b $\bar{3}$.	$0,0,0$	$0,0,\frac{1}{2}$			$hkil$: $l=2n$
6 a 3 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

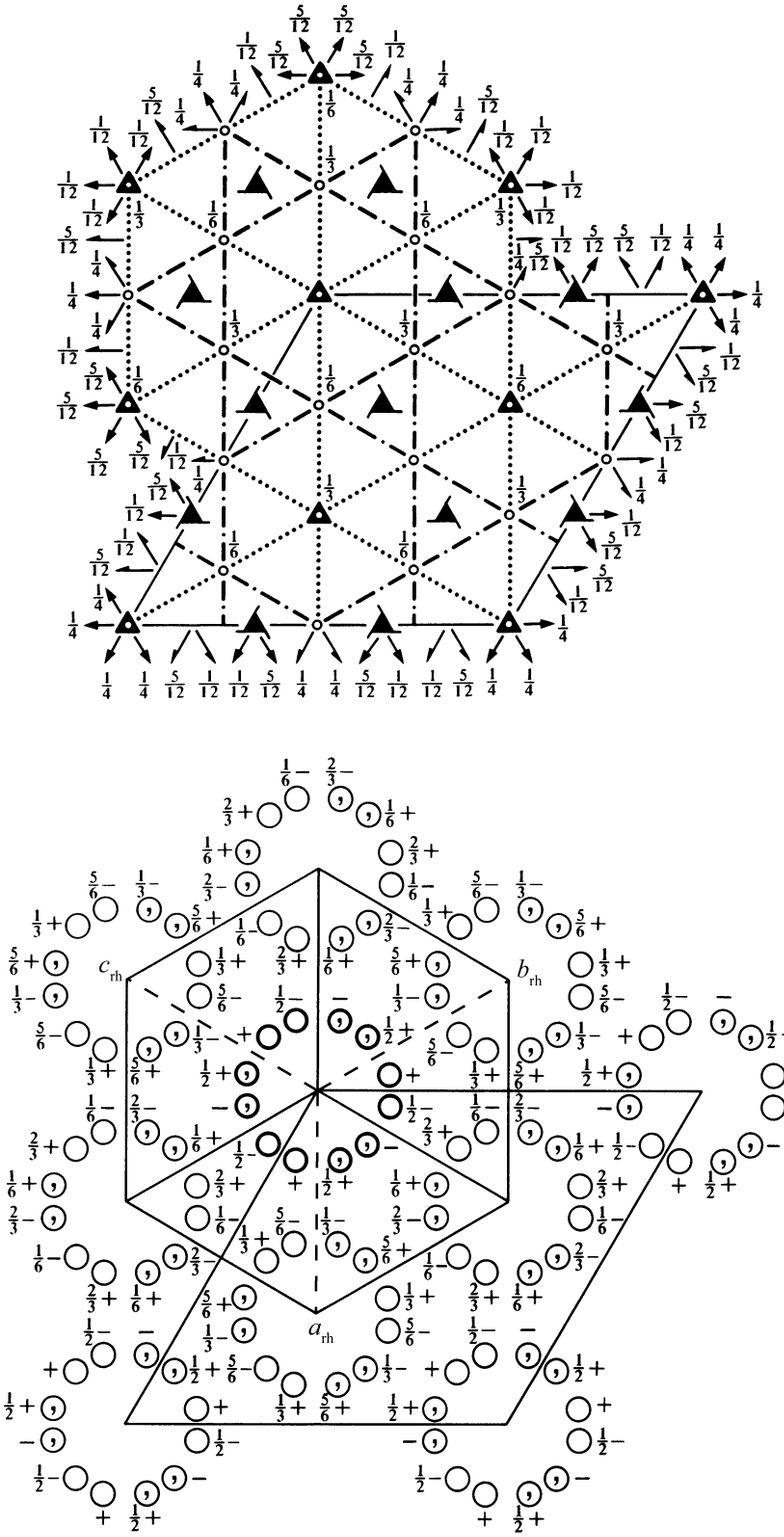
Along [100] $p2$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}+4\mathbf{b}+\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}-2\mathbf{b}+\mathbf{c})$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{3}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

No. 167 $R\bar{3}2/c$

Patterson symmetry $R\bar{3}m$

RHOMBOHEDRAL AXES



Heights refer to hexagonal axes

Origin at centre $(\bar{3})$ at $\bar{3}c$

Asymmetric unit $\frac{1}{4} \le x \le \frac{5}{4}; \quad \frac{1}{4} \le y \le \frac{5}{4}; \quad \frac{1}{4} \le z \le \frac{3}{4}; \quad y \le x; \quad z \le \min(y, \frac{3}{2} - x)$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4} \quad \frac{5}{4},\frac{1}{4},\frac{1}{4} \quad \frac{5}{4},\frac{5}{4},\frac{1}{4} \quad \frac{3}{4},\frac{3}{4},\frac{3}{4}$

Symmetry operations

(1) 1	(2) 3^+ x,x,x	(3) 3^- x,x,x
(4) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$	(5) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(6) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ x,x,x; $0,0,0$	(9) $\bar{3}^-$ x,x,x; $0,0,0$
(10) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(11) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(12) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z	(2) z,x,y	(3) y,z,x	hhl: $l=2n$
			(4) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(5) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	hhh: $h=2n$
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $\bar{z},\bar{x},\bar{y}$	(9) $\bar{y},\bar{z},\bar{x}$	
			(10) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(11) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(12) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	
						Special: as above, plus
6	e	. 2	$x,\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},x,\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{4},x$	no extra conditions
			$\bar{x},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{x},x+\frac{1}{2}$	$x+\frac{1}{2},\frac{3}{4},\bar{x}$	
6	d	$\bar{1}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$ $0,0,\frac{1}{2}$ $0,\frac{1}{2},0$ hkl: $h+k+l=2n$
4	c	3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ hkl: $h+k+l=2n$
2	b	$\bar{3}$.	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		hkl: $h+k+l=2n$
2	a	3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$		hkl: $h+k+l=2n$

Symmetry of special projections

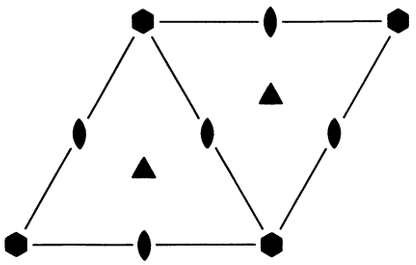
Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

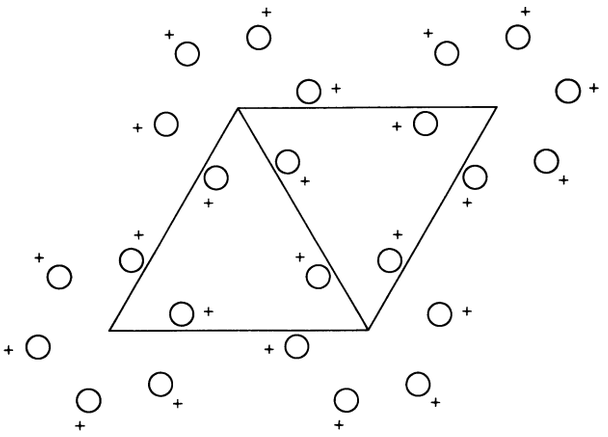
Along [1$\bar{1}$0] $p2$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+\mathbf{b}-2\mathbf{c})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\bar{x},0$

Along [2$\bar{1}\bar{1}$] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Origin at $2x,\bar{x},\bar{x}$

$P6$ C_6^1 6 Hexagonal

No. 168 $P6$ Patterson symmetry $P6/m$





Origin on 6

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$ $\frac{1}{2},\frac{1}{2},1$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) 2 $0,0,z$ (5) 6^- $0,0,z$ (6) 6^+ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6 d 1		(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
		(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
					Special: no extra conditions
3 c 2 . .		$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	
2 b 3 . .		$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$		
1 a 6 . .		$0,0,z$			

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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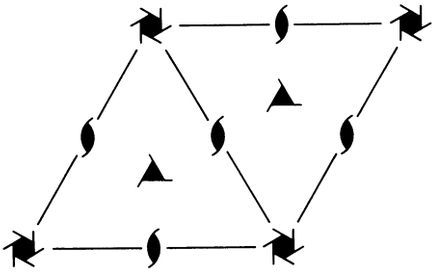
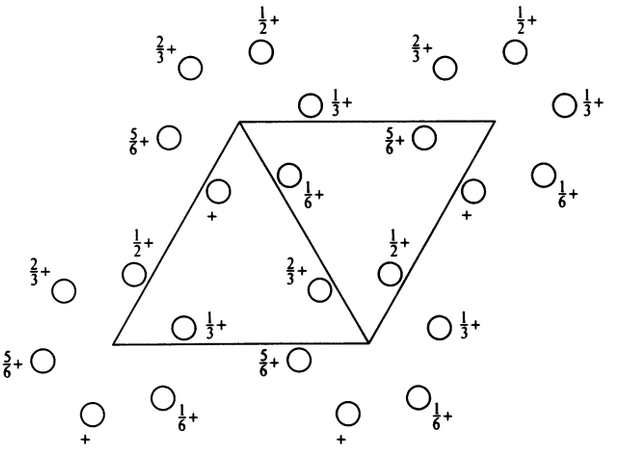
Hexagonal 6 C_6^2 $P6_1$

Patterson symmetry $P6/m$ $P6_1$ No. 169





Origin on 6_1

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le 1; \quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$
$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$ (5) $6^-(0,0,\frac{5}{6})$ $0,0,z$ (6) $6^+(0,0,\frac{1}{6})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates		Reflection conditions
				General:
6 a 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$	

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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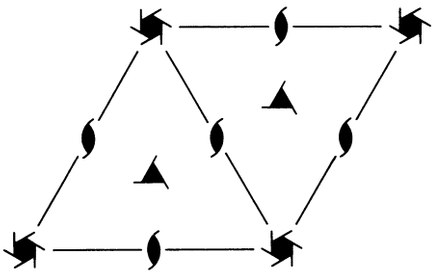
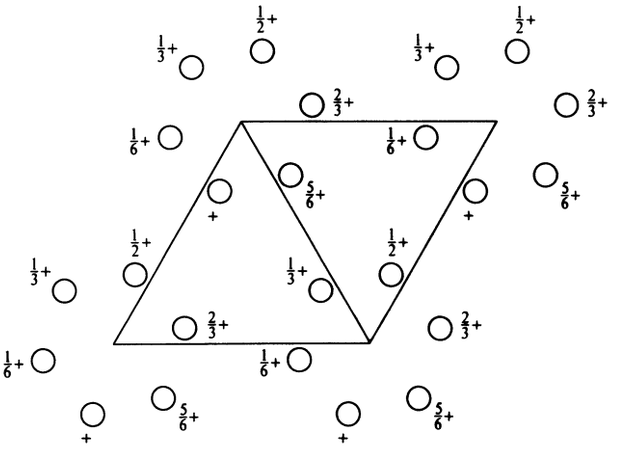
$P6_5$ C_6^3 6 Hexagonal

No. 170 $P6_5$ Patterson symmetry $P6/m$





Origin on 6_5

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{6} \quad 1,0,\frac{1}{6} \quad 1,1,\frac{1}{6} \quad 0,1,\frac{1}{6}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$

(4) $2(0,0,\frac{1}{2})$ $0,0,z$ (5) $6^-(0,0,\frac{1}{6})$ $0,0,z$ (6) $6^+(0,0,\frac{5}{6})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 a 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$	

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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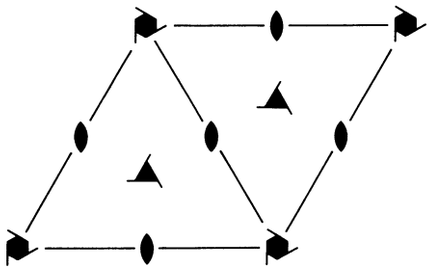
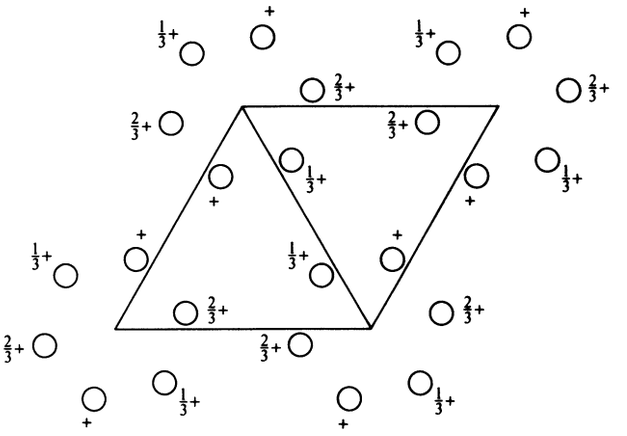
Hexagonal 6 C_6^4 $P6_2$

Patterson symmetry $P6/m$ $P6_2$ No. 171





Origin on 2 on 6_2

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{3}$; $y \le x$

Vertices $0,0,0$ $1,0,0$ $1,1,0$
$0,0,\frac{1}{3}$ $1,0,\frac{1}{3}$ $1,1,\frac{1}{3}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{2}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
(4) 2 $0,0,z$ (5) $6^-(0,0,\frac{2}{3})$ $0,0,z$ (6) $6^+(0,0,\frac{1}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	*c*	1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l$: $l=3n$
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{2}{3}$	(6) $x-y,x,z+\frac{1}{3}$	
						Special: as above, plus
3	*b*	2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{2}{3}$	$0,\frac{1}{2},z+\frac{1}{3}$	*hkil*: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	*a*	2 . .	$0,0,z$	$0,0,z+\frac{2}{3}$	$0,0,z+\frac{1}{3}$	*hkil*: $l=3n$

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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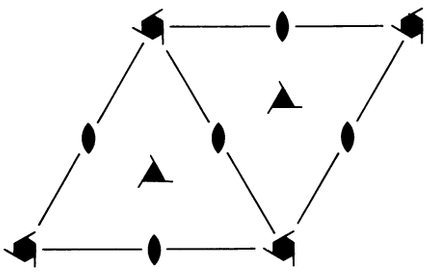
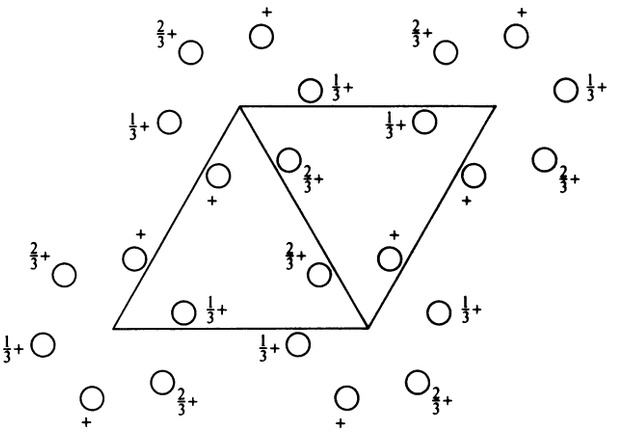
$P6_4$ C_6^5 6 Hexagonal

No. 172 $P6_4$ Patterson symmetry $P6/m$





Origin on 2 on 6_4

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{3};\quad y \le x$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0$
$0,0,\frac{1}{3}\quad 1,0,\frac{1}{3}\quad 1,1,\frac{1}{3}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
(4) 2 $0,0,z$ (5) $6^-(0,0,\frac{1}{3})$ $0,0,z$ (6) $6^+(0,0,\frac{2}{3})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			Reflection conditions
					General:
6	*c* 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l$: $l=3n$
		(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z+\frac{1}{3}$	(6) $x-y,x,z+\frac{2}{3}$	
					Special: as above, plus
3	*b* 2 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,z+\frac{1}{3}$	$0,\frac{1}{2},z+\frac{2}{3}$	$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	*a* 2 . .	$0,0,z$	$0,0,z+\frac{1}{3}$	$0,0,z+\frac{2}{3}$	$hkil$: $l=3n$

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}\quad \mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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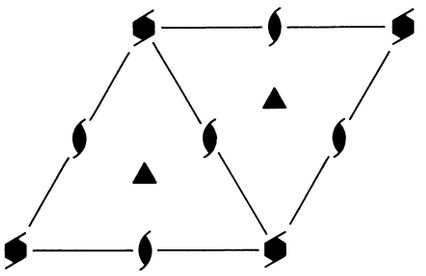
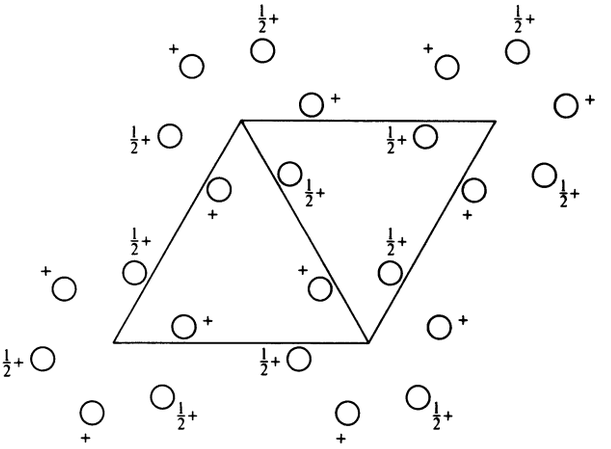
Hexagonal 6 C_6^6 $P6_3$

Patterson symmetry $P6/m$ $P6_3$ No. 173





Origin on 3 on 6_3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$ (5) $6^-(0,0,\frac{1}{2})$ $0,0,z$ (6) $6^+(0,0,\frac{1}{2})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	$000l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$	
						Special: as above, plus
2	b	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$		$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	a	3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$		$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,g\,1$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p\,1\,g\,1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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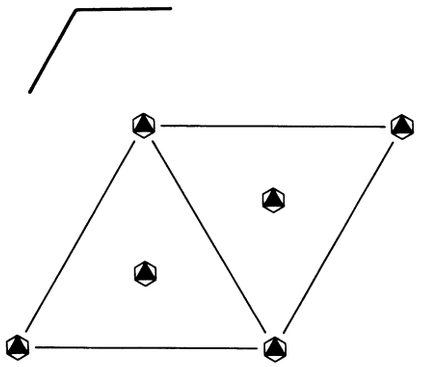
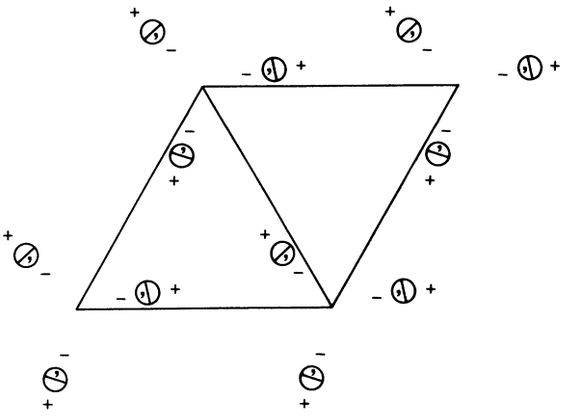
$P\bar{6}$ C_{3h}^{1} $\bar{6}$ Hexagonal

No. 174 $P\bar{6}$ Patterson symmetry $P6/m$





Origin at $\bar{6}$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$ $0,\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^+ $0,0,z$ (3) 3^- $0,0,z$
(4) m $x,y,0$ (5) $\bar{6}^-$ $0,0,z$; $0,0,0$ (6) $\bar{6}^+$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$	
						Special: no extra conditions
3	k	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	
3	j	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	
2	i	3 . .	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	h	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	g	3 . .	$0,0,z$	$0,0,\bar{z}$		
1	f	$\bar{6}$ . .	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$			
1	e	$\bar{6}$ . .	$\frac{2}{3},\frac{1}{3},0$			
1	d	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			
1	c	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},0$			
1	b	$\bar{6}$ . .	$0,0,\frac{1}{2}$			
1	a	$\bar{6}$ . .	$0,0,0$			

Symmetry of special projections

Along [001] $p3$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,1\,1\,m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p\,1\,1\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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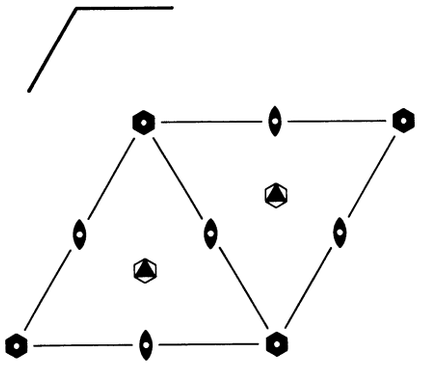
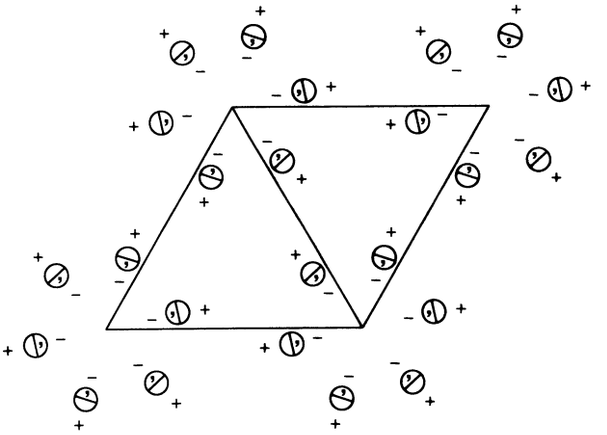
Hexagonal $6/m$ C_{6h}^{1} $P6/m$

Patterson symmetry $P6/m$ $P6/m$ No. 175





Origin at centre $(6/m)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $0,0,z$	(5) 6^- $0,0,z$	(6) 6^+ $0,0,z$
(7) $\bar{1}$ $0,0,0$	(8) $\bar{3}^+$ $0,0,z$; $0,0,0$	(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) m $x,y,0$	(11) $\bar{6}^-$ $0,0,z$; $0,0,0$	(12) $\bar{6}^+$ $0,0,z$; $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
12 l 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
	(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	
	(10) $x,y,\bar{z}$	(11) $\bar{y},x-y,\bar{z}$	(12) $\bar{x}+y,\bar{x},\bar{z}$	
				Special: no extra conditions
6 k m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$y,\bar{x}+y,\frac{1}{2}$	$x-y,x,\frac{1}{2}$
6 j m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{x},\bar{y},0$	$y,\bar{x}+y,0$	$x-y,x,0$
6 i 2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$
4 h 3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
3 g $2/m$ . .	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
3 f $2/m$ . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2 e 6 . .	$0,0,z$	$0,0,\bar{z}$				
2 d $\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$				
2 c $\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$				
1 b $6/m$ . .	$0,0,\frac{1}{2}$					
1 a $6/m$ . .	$0,0,0$					

Symmetry of special projections

Along [001] $p6$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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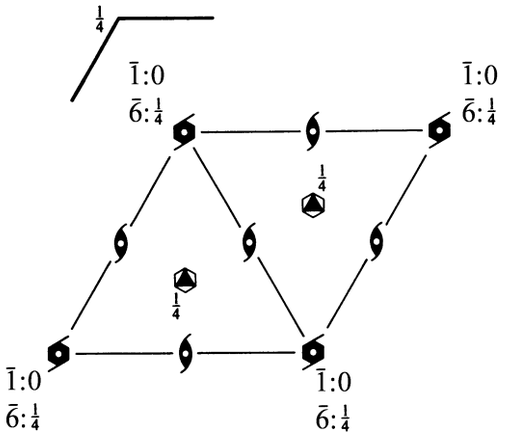
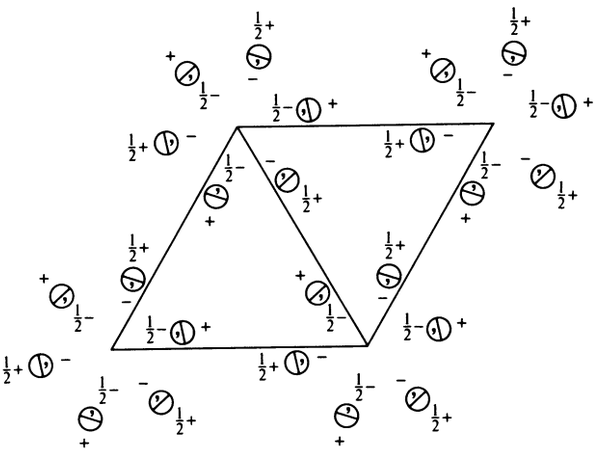
$P6_3/m$ C_{6h}^2 $6/m$ Hexagonal

No. 176 $P6_3/m$ Patterson symmetry $P6/m$





Origin at centre $(\bar{3})$ on 6_3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$
(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$
(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) $\bar{1}$ $0,0,0$
(8) $\bar{3}^+$ $0,0,z$; $0,0,0$
(9) $\bar{3}^-$ $0,0,z$; $0,0,0$
(10) m $x,y,\frac{1}{4}$
(11) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$
(12) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z (4) $\bar{x},\bar{y},z+\frac{1}{2}$ (7) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z+\frac{1}{2}$ (8) $y,\bar{x}+y,\bar{z}$ (11) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z+\frac{1}{2}$ (9) $x-y,x,\bar{z}$ (12) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				$000l$: $l=2n$
									Special: as above, plus
6	h	m . .	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
6	g	$\bar{1}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	f	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$
2	d	$\bar{6}$ . .	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	b	$\bar{3}$ . .	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	$\bar{6}$ . .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

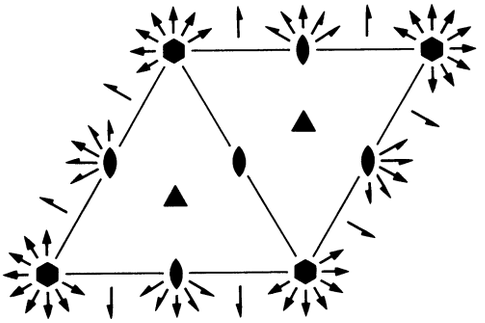
Along [001] $p6$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

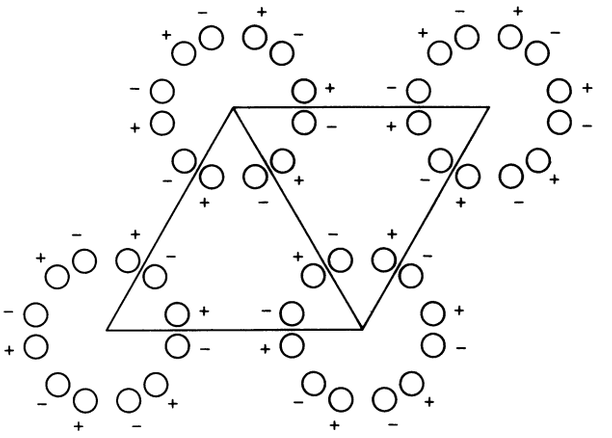
Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P622$ D_6^1 622 Hexagonal

No. 177 $P622$ Patterson symmetry $P6/mmm$





Origin at 622

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) 2 $0,0,z$
(5) 6^- $0,0,z$
(6) 6^+ $0,0,z$
(7) 2 $x,x,0$
(8) 2 $x,0,0$
(9) 2 $0,y,0$
(10) 2 $x,\bar{x},0$
(11) 2 $x,2x,0$
(12) 2 $2x,x,0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	n	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}$ (10) $\bar{y},\bar{x},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $\bar{x},\bar{x}+y,\bar{z}$ (12) $x,x-y,\bar{z}$				no conditions
									Special: no extra conditions
6	m	. . 2	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	
6	l	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$\bar{x},x,0$	$\bar{x},2\bar{x},0$	$2x,x,0$	
6	k	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	
6	j	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	
6	i	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$	
4	h	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			
3	g	2 2 2	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
3	f	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$				
2	e	6 . .	$0,0,z$	$0,0,\bar{z}$					
2	d	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	3 . 2	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	6 2 2	$0,0,\frac{1}{2}$						
1	a	6 2 2	$0,0,0$						

Symmetry of special projections

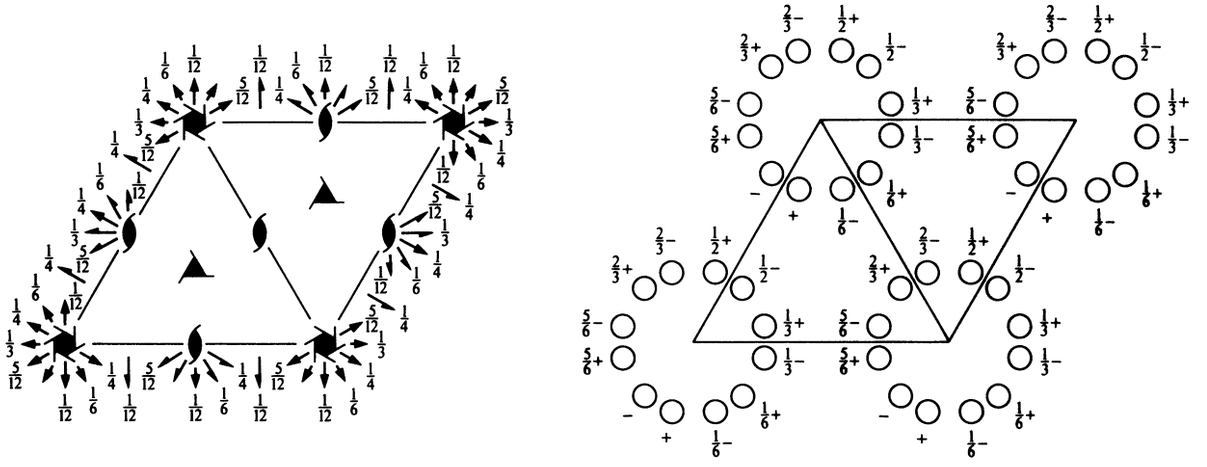
Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P6_122$ D_6^2 622 Hexagonal

No. 178 $P6_122$ Patterson symmetry $P6/mmm$



Origin on $2[100]$ at $6_1\,(2,1,1)\,1$

Asymmetric unit $0 \le x \le 1$; $0 \le y \le 1$; $0 \le z \le \frac{1}{12}$

Vertices $0,0,0$ $1,0,0$ $1,1,0$ $0,1,0$
$0,0,\frac{1}{12}$ $1,0,\frac{1}{12}$ $1,1,\frac{1}{12}$ $0,1,\frac{1}{12}$

Symmetry operations

(1) 1 (2) $3^+(0,0,\frac{1}{3})$ $0,0,z$ (3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$ (5) $6^-(0,0,\frac{5}{6})$ $0,0,z$ (6) $6^+(0,0,\frac{1}{6})$ $0,0,z$
(7) 2 $x,x,\frac{1}{6}$ (8) 2 $x,0,0$ (9) 2 $0,y,\frac{1}{3}$
(10) 2 $x,\bar{x},\frac{5}{12}$ (11) 2 $x,2x,\frac{1}{4}$ (12) 2 $2x,x,\frac{1}{12}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
12 c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$	
	(7) $y,x,\bar{z}+\frac{1}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$	
	(10) $\bar{y},\bar{x},\bar{z}+\frac{5}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{6}$	
				Special: as above, plus
6 b . . 2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{7}{12}$	$x,\bar{x},\frac{11}{12}$	$\bar{x},2\bar{x},\frac{3}{4}$ $2x,x,\frac{1}{12}$ $\bar{x},x,\frac{5}{12}$	$hh\overline{2h}l$: $l=2n$ or $l=3n+1$ or $l=3n+2$
6 a . 2 .	$x,0,0$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},\frac{2}{3}$	$\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{5}{6}$ $x,x,\frac{1}{6}$	$hh\bar{0}l$: $l=2n$ or $l=3n+1$ or $l=3n+2$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{12}$

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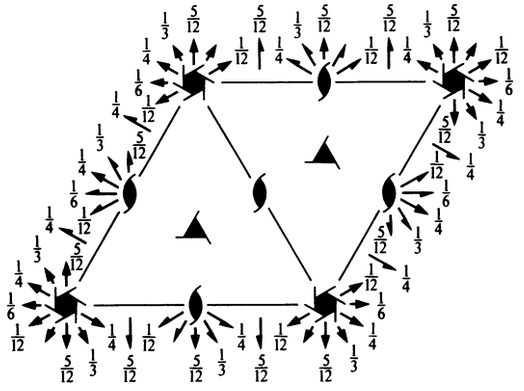
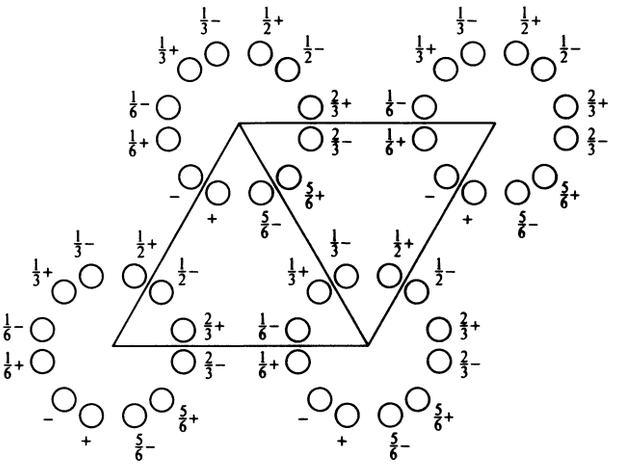
Hexagonal 622 D_6^3 $P6_522$

Patterson symmetry $P6/mmm$ $P6_522$ No. 179





Origin on $2[100]$ at $6_5\,(2,1,1)\,1$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{12}$

Vertices $0,0,0 \quad 1,0,0 \quad 1,1,0 \quad 0,1,0$

$0,0,\frac{1}{12} \quad 1,0,\frac{1}{12} \quad 1,1,\frac{1}{12} \quad 0,1,\frac{1}{12}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{1}{6})$ $0,0,z$	(6) $6^+(0,0,\frac{5}{6})$ $0,0,z$
(7) 2 $x,x,\frac{1}{3}$	(8) 2 $x,0,0$	(9) 2 $0,y,\frac{1}{6}$
(10) 2 $x,\bar{x},\frac{1}{12}$	(11) 2 $x,2x,\frac{1}{4}$	(12) 2 $2x,x,\frac{5}{12}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
12 c 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{2}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$	$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{6}$	(6) $x-y,x,z+\frac{5}{6}$	
	(7) $y,x,\bar{z}+\frac{2}{3}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$	
	(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{6}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{5}{6}$	
				Special: as above, plus
6 b . . 2	$x,2x,\frac{3}{4}$	$2\bar{x},\bar{x},\frac{5}{12}$	$x,\bar{x},\frac{1}{12}$	$\bar{x},2\bar{x},\frac{1}{4}$ $2x,x,\frac{11}{12}$ $\bar{x},x,\frac{7}{12}$	$hh\overline{2h}l$: $l=2n$ or $l=3n+1$ or $l=3n+2$
6 a . 2 .	$x,0,0$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},\frac{1}{3}$	$\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{1}{6}$ $x,x,\frac{5}{6}$	$h\bar{h}0l$: $l=2n$ or $l=3n+1$ or $l=3n+2$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{5}{12}$

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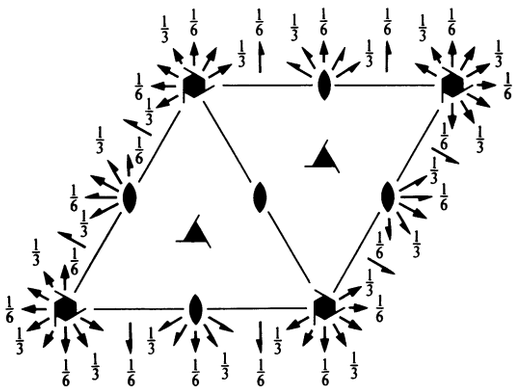
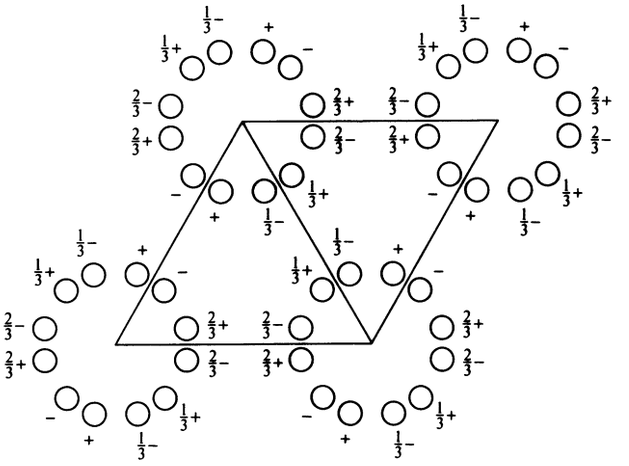
$P6_222$ D_6^4 622 Hexagonal

No. 180 $P6_222$ Patterson symmetry $P6/mmm$





Origin at 222 at $6_2\,(2,1,1)\,(1,2,1)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6};\quad y \le x$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0$

$0,0,\frac{1}{6}\quad 1,0,\frac{1}{6}\quad 1,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{2}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{1}{3})$ $0,0,z$
(4) 2 $0,0,z$	(5) $6^-(0,0,\frac{2}{3})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{3})$ $0,0,z$
(7) 2 $x,x,\frac{1}{3}$	(8) 2 $x,0,0$	(9) 2 $0,y,\frac{1}{6}$
(10) 2 $x,\bar{x},\frac{1}{3}$	(11) 2 $x,2x,0$	(12) 2 $2x,x,\frac{1}{6}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	k	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}+\frac{2}{3}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{2}{3}$	(2) $\bar{y},x-y,z+\frac{2}{3}$ (5) $y,\bar{x}+y,z+\frac{2}{3}$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$ (6) $x-y,x,z+\frac{1}{3}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{3}$ (12) $x,x-y,\bar{z}+\frac{1}{3}$				$000l$: $l=3n$
									Special: as above, plus
6	j	. . 2	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{6}$	$x,\bar{x},\frac{5}{6}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{6}$	$\bar{x},x,\frac{5}{6}$	no extra conditions
6	i	. . 2	$x,2x,0$	$2\bar{x},\bar{x},\frac{2}{3}$	$x,\bar{x},\frac{1}{3}$	$\bar{x},2\bar{x},0$	$2x,x,\frac{2}{3}$	$\bar{x},x,\frac{1}{3}$	no extra conditions
6	h	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{6}$	$\bar{x},\bar{x},\frac{5}{6}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{6}$	$x,x,\frac{5}{6}$	no extra conditions
6	g	. 2 .	$x,0,0$	$0,x,\frac{2}{3}$	$\bar{x},\bar{x},\frac{1}{3}$	$\bar{x},0,0$	$0,\bar{x},\frac{2}{3}$	$x,x,\frac{1}{3}$	no extra conditions
6	f	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{2}{3}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{3}$	$0,\frac{1}{2},\bar{z}+\frac{2}{3}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{3}$	$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
6	e	2 . .	$0,0,z$	$0,0,z+\frac{2}{3}$	$0,0,z+\frac{1}{3}$	$0,0,\bar{z}+\frac{2}{3}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{3}$	$hkil$: $l=3n$
3	d	2 2 2	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{6}$	$\frac{1}{2},\frac{1}{2},\frac{5}{6}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	c	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{2}{3}$	$\frac{1}{2},\frac{1}{2},\frac{1}{3}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	b	2 2 2	$0,0,\frac{1}{2}$	$0,0,\frac{1}{6}$	$0,0,\frac{5}{6}$				$hkil$: $l=3n$
3	a	2 2 2	$0,0,0$	$0,0,\frac{2}{3}$	$0,0,\frac{1}{3}$				$hkil$: $l=3n$

Symmetry of special projections

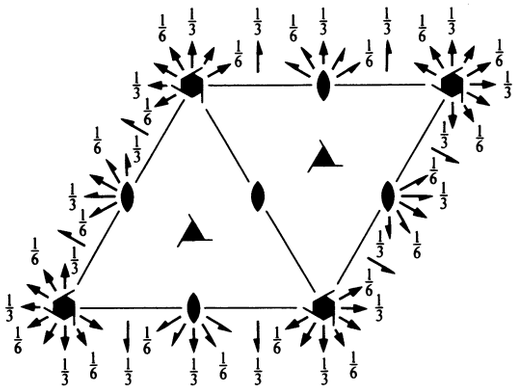
Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

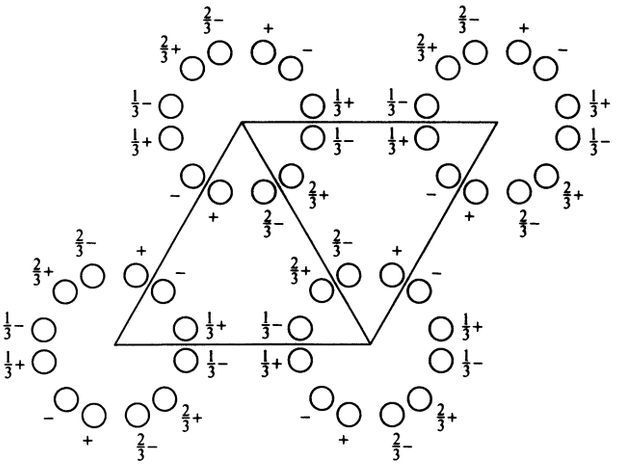
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{6}$

$P6_422$ D_6^5 622 Hexagonal

No. 181 $P6_422$ Patterson symmetry $P6/mmm$





Origin at 222 at $6_4\,(2,1,1)\,(1,2,1)$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{6};\quad y \le x$

Vertices $0,0,0\quad 1,0,0\quad 1,1,0$

$0,0,\frac{1}{6}\quad 1,0,\frac{1}{6}\quad 1,1,\frac{1}{6}$

Symmetry operations

(1) 1	(2) $3^+(0,0,\frac{1}{3})$ $0,0,z$	(3) $3^-(0,0,\frac{2}{3})$ $0,0,z$
(4) 2 $0,0,z$	(5) $6^-(0,0,\frac{1}{3})$ $0,0,z$	(6) $6^+(0,0,\frac{2}{3})$ $0,0,z$
(7) 2 $x,x,\frac{1}{6}$	(8) 2 $x,0,0$	(9) 2 $0,y,\frac{1}{3}$
(10) 2 $x,\bar{x},\frac{1}{6}$	(11) 2 $x,2x,0$	(12) 2 $2x,x,\frac{1}{3}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	k	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}+\frac{1}{3}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{1}{3}$	(2) $\bar{y},x-y,z+\frac{1}{3}$ (5) $y,\bar{x}+y,z+\frac{1}{3}$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$ (6) $x-y,x,z+\frac{2}{3}$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$ (12) $x,x-y,\bar{z}+\frac{2}{3}$				$000l$: $l=3n$
									Special: as above, plus
6	j	. . 2	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{5}{6}$	$x,\bar{x},\frac{1}{6}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{5}{6}$	$\bar{x},x,\frac{1}{6}$	no extra conditions
6	i	. . 2	$x,2x,0$	$2\bar{x},\bar{x},\frac{1}{3}$	$x,\bar{x},\frac{2}{3}$	$\bar{x},2\bar{x},0$	$2x,x,\frac{1}{3}$	$\bar{x},x,\frac{2}{3}$	no extra conditions
6	h	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{5}{6}$	$\bar{x},\bar{x},\frac{1}{6}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{5}{6}$	$x,x,\frac{1}{6}$	no extra conditions
6	g	. 2 .	$x,0,0$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},\frac{2}{3}$	$\bar{x},0,0$	$0,\bar{x},\frac{1}{3}$	$x,x,\frac{2}{3}$	no extra conditions
6	f	2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z+\frac{1}{3}$	$\frac{1}{2},\frac{1}{2},z+\frac{2}{3}$	$0,\frac{1}{2},\bar{z}+\frac{1}{3}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{2}{3}$	$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
6	e	2 . .	$0,0,z$	$0,0,z+\frac{1}{3}$	$0,0,z+\frac{2}{3}$	$0,0,\bar{z}+\frac{1}{3}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{2}{3}$	$hkil$: $l=3n$
3	d	2 2 2	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{5}{6}$	$\frac{1}{2},\frac{1}{2},\frac{1}{6}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	c	2 2 2	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{3}$	$\frac{1}{2},\frac{1}{2},\frac{2}{3}$				$hkil$: $h=2n+1$ or $k=2n+1$ or $l=3n$
3	b	2 2 2	$0,0,\frac{1}{2}$	$0,0,\frac{5}{6}$	$0,0,\frac{1}{6}$				$hkil$: $l=3n$
3	a	2 2 2	$0,0,0$	$0,0,\frac{1}{3}$	$0,0,\frac{2}{3}$				$hkil$: $l=3n$

Symmetry of special projections

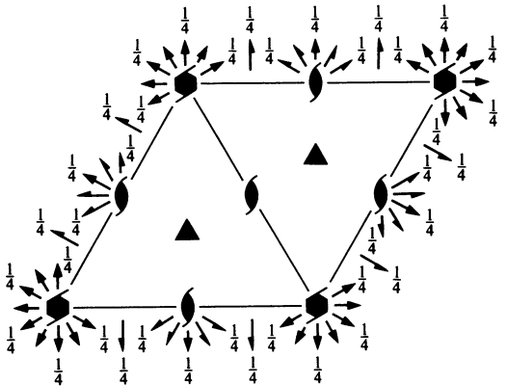
Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

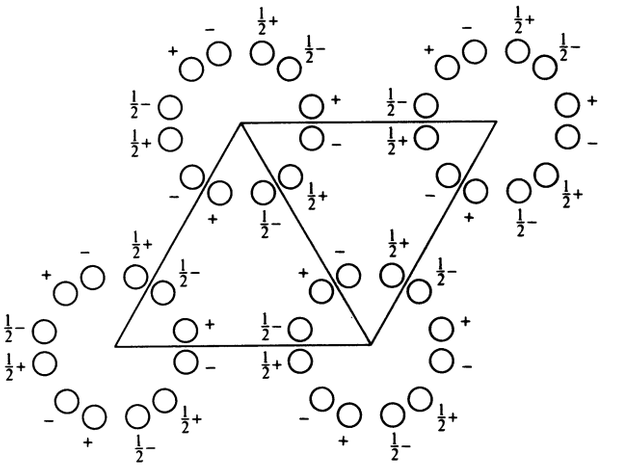
Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{3}$

$P6_322$ D_6^6 622 Hexagonal

No. 182 $P6_322$ Patterson symmetry $P6/mmm$





Origin at 321 at $6_3 21$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$
(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$
(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) 2 $x,x,0$
(8) 2 $x,0,0$
(9) 2 $0,y,0$
(10) 2 $x,\bar{x},\frac{1}{4}$
(11) 2 $x,2x,\frac{1}{4}$
(12) 2 $2x,x,\frac{1}{4}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z (4) $\bar{x},\bar{y},z+\frac{1}{2}$ (7) $y,x,\bar{z}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z+\frac{1}{2}$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z+\frac{1}{2}$ (9) $\bar{x},\bar{x}+y,\bar{z}$ (12) $x,x-y,\bar{z}+\frac{1}{2}$				$000l$: $l=2n$
									Special: as above, plus
6	h	. . 2	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	$hh\overline{2h}l$: $l=2n$
6	g	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	$h\bar{h}0l$: $l=2n$
4	f	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	3 . .	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$
2	d	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	b	3 . 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	3 2 .	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

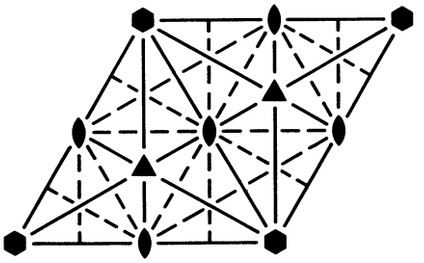
Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

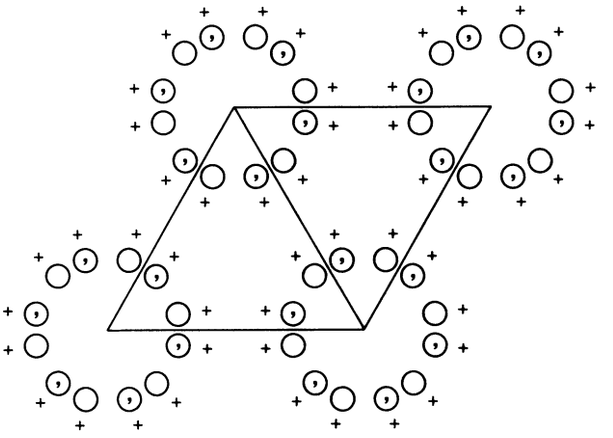
Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,\frac{1}{4}$

$P6mm$ C_{6v}^{1} $6mm$ Hexagonal

No. 183 $P6mm$ Patterson symmetry $P6/mmm$





Origin on $6mm$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$
$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $0,0,z$	(5) 6^- $0,0,z$	(6) 6^+ $0,0,z$
(7) m $x,\bar{x},z$	(8) m $x,2x,z$	(9) m $2x,x,z$
(10) m x,x,z	(11) m $x,0,z$	(12) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	f	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$	
			(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$	
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$	
						Special: no extra conditions
6	e	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z$ $\bar{x},2\bar{x},z$ $2x,x,z$
6	d	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z$ $0,\bar{x},z$ x,x,z
3	c	2 m m	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	
2	b	3 m .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$		
1	a	6 m m	$0,0,z$			

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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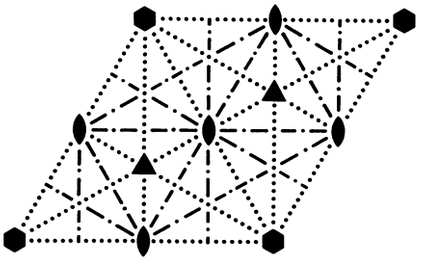
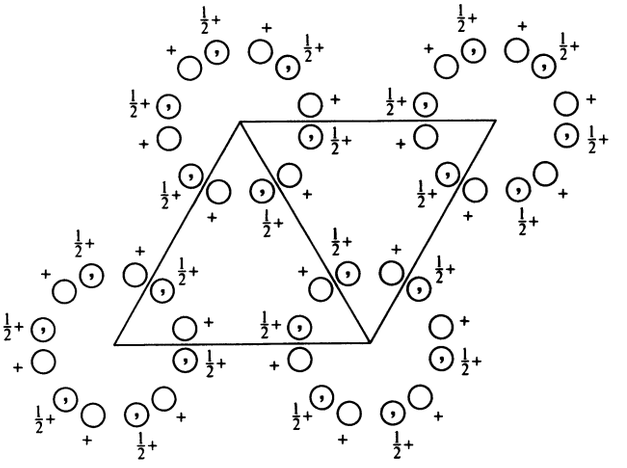
Hexagonal $6mm$ C_{6v}^2 $P6cc$

Patterson symmetry $P6/mmm$ $P6cc$ No. 184





Origin on $6cc$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $0,0,z$	(5) 6^- $0,0,z$	(6) 6^+ $0,0,z$
(7) c $x,\bar{x},z$	(8) c $x,2x,z$	(9) c $2x,x,z$
(10) c x,x,z	(11) c $x,0,z$	(12) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
							General:
12 d 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$
	(4) $\bar{x},\bar{y},z$	(5) $y,\bar{x}+y,z$	(6) $x-y,x,z$				$h\bar{h}0l$: $l=2n$
	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$				$000l$: $l=2n$
	(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
							Special: as above, plus
6 c 2 . .	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$hkil$: $l=2n$
4 b 3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$			$hkil$: $l=2n$
2 a 6 . .	$0,0,z$	$0,0,z+\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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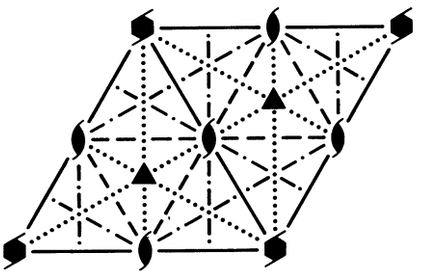
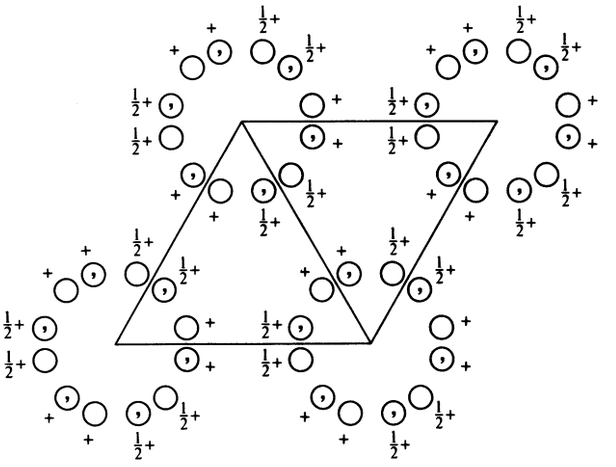
$P6_3cm$ C_{6v}^3 $6mm$ Hexagonal

No. 185 $P6_3cm$ Patterson symmetry $P6/mmm$





Origin on $31m$ on 6_3cm

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) c $x,\bar{x},z$	(8) c $x,2x,z$	(9) c $2x,x,z$
(10) m x,x,z	(11) m $x,0,z$	(12) m $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
							General:
12 d 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$h\bar{h}0l$: $l=2n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				$000l$: $l=2n$
	(7) $\bar{y},\bar{x},z+\frac{1}{2}$	(8) $\bar{x}+y,y,z+\frac{1}{2}$	(9) $x,x-y,z+\frac{1}{2}$				
	(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$				
							Special: as above, plus
6 c $..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z+\frac{1}{2}$	$0,\bar{x},z+\frac{1}{2}$	$x,x,z+\frac{1}{2}$	no extra conditions
4 b 3..	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z$			$hkil$: $l=2n$
2 a $3.m$	$0,0,z$	$0,0,z+\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1m1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1g1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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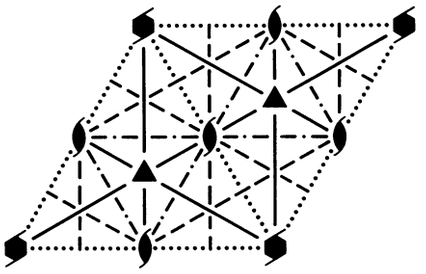
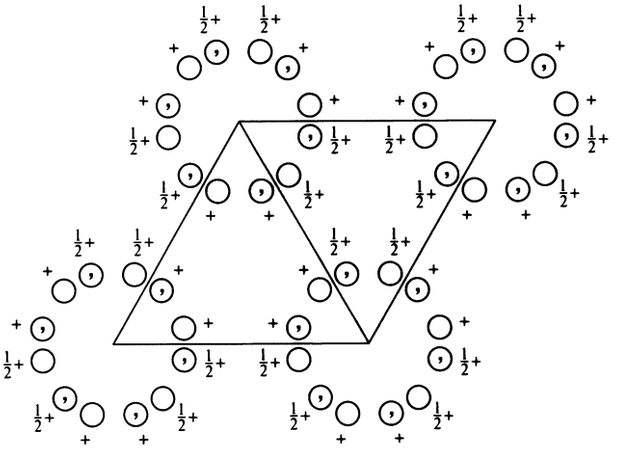
Hexagonal $6mm$ C_{6v}^4 $P6_3mc$

Patterson symmetry $P6/mmm$ $P6_3mc$ No. 186





Origin on $3m1$ on 6_3mc

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $0 \le z \le 1$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$
$0,0,1$ $\frac{1}{2},0,1$ $\frac{2}{3},\frac{1}{3},1$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$	(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$	(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) m $x,\bar{x},z$	(8) m $x,2x,z$	(9) m $2x,x,z$
(10) c x,x,z	(11) c $x,0,z$	(12) c $0,y,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
							General:
12 d 1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				$000l$: $l=2n$
	(7) $\bar{y},\bar{x},z$	(8) $\bar{x}+y,y,z$	(9) $x,x-y,z$				
	(10) $y,x,z+\frac{1}{2}$	(11) $x-y,\bar{y},z+\frac{1}{2}$	(12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
							Special: as above, plus
6 c . m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,z+\frac{1}{2}$	$\bar{x},2\bar{x},z+\frac{1}{2}$	$2x,x,z+\frac{1}{2}$	no extra conditions
2 b $3m$.	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2 a $3m$.	$0,0,z$	$0,0,z+\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p1g1$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p1m1$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

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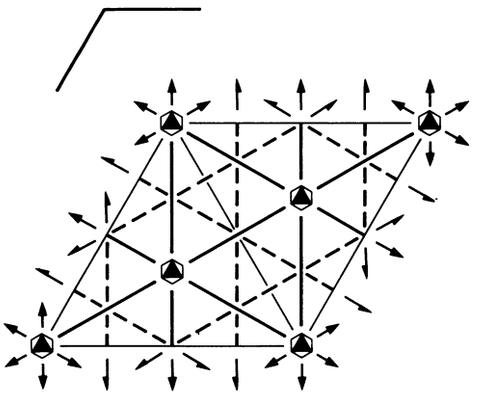
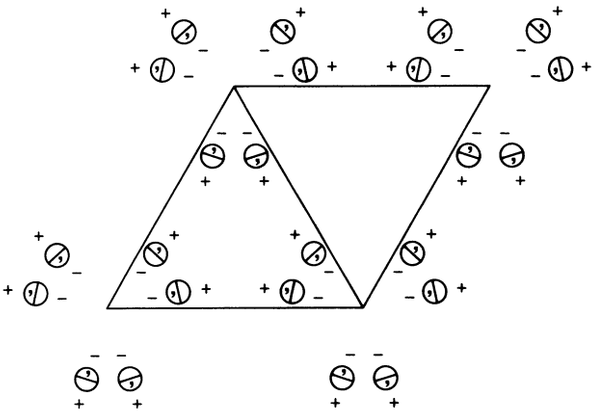
$P\bar{6}m2$ D_{3h}^{1} $\bar{6}m2$ Hexagonal

No. 187 $P\bar{6}m2$ Patterson symmetry $P6/mmm$





Origin at $\bar{6}m2$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{2}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$
$0,0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) m $x,y,0$	(5) $\bar{6}^-$ $0,0,z$; $0,0,0$	(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
(7) m $x,\bar{x},z$	(8) m $x,2x,z$	(9) m $2x,x,z$
(10) 2 $x,\bar{x},0$	(11) 2 $x,2x,0$	(12) 2 $2x,x,0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	o	1	(1) x,y,z (4) $x,y,\bar{z}$ (7) $\bar{y},\bar{x},z$ (10) $\bar{y},\bar{x},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}$ (8) $\bar{x}+y,y,z$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}$ (9) $x,x-y,z$ (12) $x,x-y,\bar{z}$	no conditions
						Special: no extra conditions
6	n	. m .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},\bar{z}$ $x,2x,\bar{z}$ $2\bar{x},\bar{x},\bar{z}$
6	m	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$\bar{y},\bar{x},\frac{1}{2}$ $\bar{x}+y,y,\frac{1}{2}$ $x,x-y,\frac{1}{2}$
6	l	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$\bar{y},\bar{x},0$ $\bar{x}+y,y,0$ $x,x-y,0$
3	k	$m\,m\,2$	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	
3	j	$m\,m\,2$	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	
2	i	$3\,m$.	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$		
2	h	$3\,m$.	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
2	g	$3\,m$.	$0,0,z$	$0,0,\bar{z}$		
1	f	$\bar{6}\,m\,2$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$			
1	e	$\bar{6}\,m\,2$	$\frac{2}{3},\frac{1}{3},0$			
1	d	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			
1	c	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},0$			
1	b	$\bar{6}\,m\,2$	$0,0,\frac{1}{2}$			
1	a	$\bar{6}\,m\,2$	$0,0,0$			

Symmetry of special projections

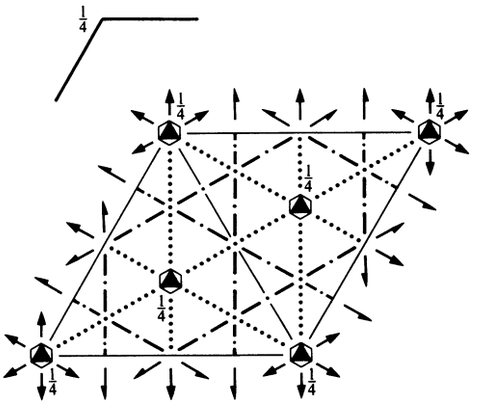
Along [001] $p\,3\,m\,1$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

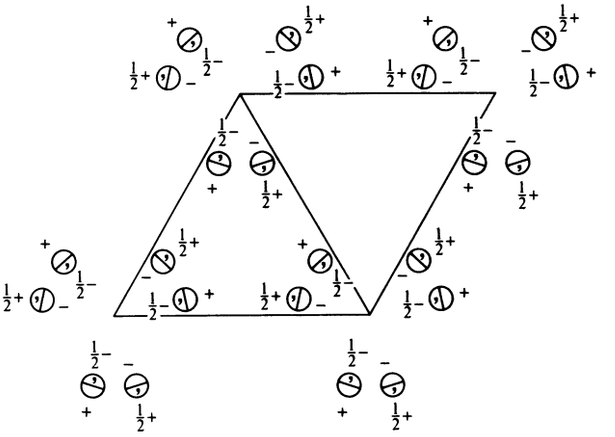
Along [100] $p\,1\,1\,m$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p\,2\,m\,m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P\bar{6}c2$ D_{3h}^2 $\bar{6}m2$ Hexagonal

No. 188 $P\bar{6}c2$ Patterson symmetry $P6/mmm$





Origin at $3c2$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) m $x,y,\frac{1}{4}$
(5) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$
(6) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(7) c $x,\bar{x},z$
(8) c $x,2x,z$
(9) c $2x,x,z$
(10) 2 $x,\bar{x},0$
(11) 2 $x,2x,0$
(12) 2 $2x,x,0$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	l	1	(1) x,y,z (4) $x,y,\bar{z}+\frac{1}{2}$ (7) $\bar{y},\bar{x},z+\frac{1}{2}$ (10) $\bar{y},\bar{x},\bar{z}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}+\frac{1}{2}$ (8) $\bar{x}+y,y,z+\frac{1}{2}$ (11) $\bar{x}+y,y,\bar{z}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$ (9) $x,x-y,z+\frac{1}{2}$ (12) $x,x-y,\bar{z}$				$h\bar{h}0l$: $l=2n$ $000l$: $l=2n$
									Special: as above, plus
6	k	m . .	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{y},\bar{x},\frac{3}{4}$	$\bar{x}+y,y,\frac{3}{4}$	$x,x-y,\frac{3}{4}$	no extra conditions
6	j	. . 2	$x,\bar{x},0$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},\frac{1}{2}$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$hkil$: $l=2n$
4	i	3 . .	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$			$hkil$: $l=2n$
4	h	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			$hkil$: $l=2n$
4	g	3 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$			$hkil$: $l=2n$
2	f	$\bar{6}$ . .	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$
2	e	3 . 2	$\frac{2}{3},\frac{1}{3},0$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					$hkil$: $l=2n$
2	d	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$					$hkil$: $l=2n$
2	c	3 . 2	$\frac{1}{3},\frac{2}{3},0$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$					$hkil$: $l=2n$
2	b	$\bar{6}$ . .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	3 . 2	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

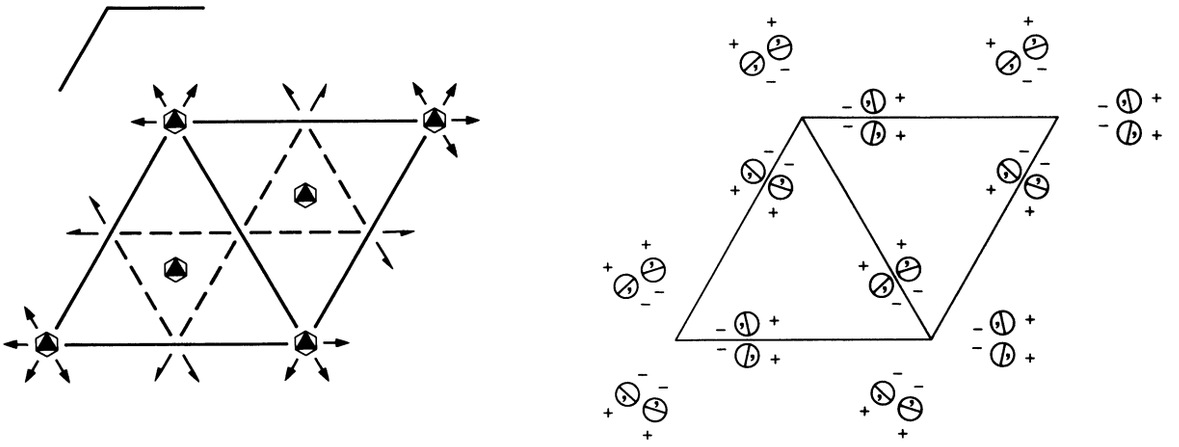
Along [001] $p3m1$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p11m$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P\bar{6}2m$ D_{3h}^3 $\bar{6}2m$ Hexagonal

No. 189 $P\bar{6}2m$ Patterson symmetry $P6/mmm$



Origin at $\bar{6}2m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) m $x,y,0$
(5) $\bar{6}^-$ $0,0,z$; $0,0,0$
(6) $\bar{6}^+$ $0,0,z$; $0,0,0$
(7) 2 $x,x,0$
(8) 2 $x,0,0$
(9) 2 $0,y,0$
(10) m x,x,z
(11) m $x,0,z$
(12) m $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				no conditions
			(4) $x,y,\bar{z}$	(5) $\bar{y},x-y,\bar{z}$	(6) $\bar{x}+y,\bar{x},\bar{z}$				
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) y,x,z	(11) $x-y,\bar{y},z$	(12) $\bar{x},\bar{x}+y,z$				
									Special: no extra conditions
6	k	m . .	$x,y,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$	$y,x,\frac{1}{2}$	$x-y,\bar{y},\frac{1}{2}$	$\bar{x},\bar{x}+y,\frac{1}{2}$	
6	j	m . .	$x,y,0$	$\bar{y},x-y,0$	$\bar{x}+y,\bar{x},0$	$y,x,0$	$x-y,\bar{y},0$	$\bar{x},\bar{x}+y,0$	
6	i	. . m	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$x,0,\bar{z}$	$0,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	
4	h	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z$			
3	g	m 2 m	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$				
3	f	m 2 m	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$				
2	e	3 . m	$0,0,z$	$0,0,\bar{z}$					
2	d	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$					
2	c	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$					
1	b	$\bar{6}$ 2 m	$0,0,\frac{1}{2}$						
1	a	$\bar{6}$ 2 m	$0,0,0$						

Symmetry of special projections

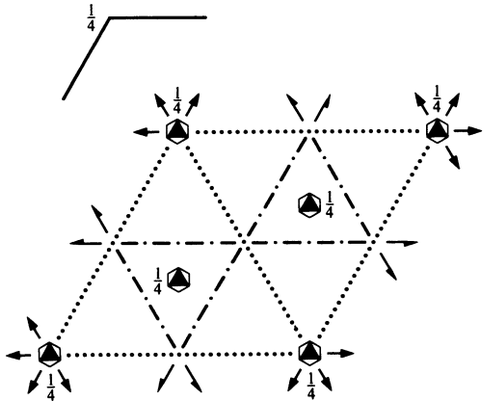
Along [001] $p31m$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

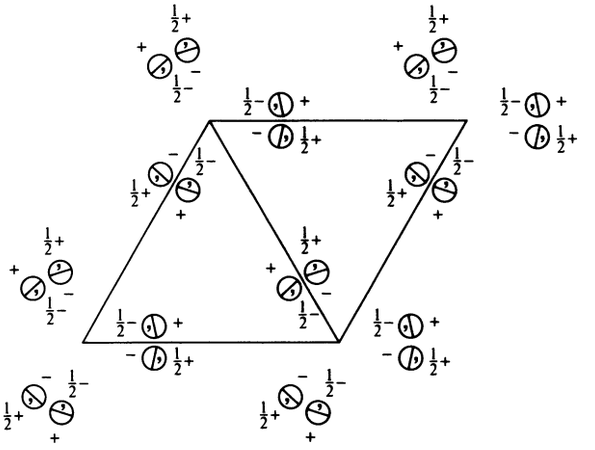
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p11m$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P\bar{6}2c$ D_{3h}^4 $\bar{6}2m$ Hexagonal

No. 190 $P\bar{6}2c$ Patterson symmetry $P6/mmm$





Origin at $32c$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$ $0,\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$ $0,\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) m $x,y,\frac{1}{4}$
(5) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$
(6) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(7) 2 $x,x,0$
(8) 2 $x,0,0$
(9) 2 $0,y,0$
(10) c x,x,z
(11) c $x,0,z$
(12) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
12	i	1	(1) x,y,z (4) $x,y,\bar{z}+\frac{1}{2}$ (7) $y,x,\bar{z}$ (10) $y,x,z+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $\bar{y},x-y,\bar{z}+\frac{1}{2}$ (8) $x-y,\bar{y},\bar{z}$ (11) $x-y,\bar{y},z+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$ (9) $\bar{x},\bar{x}+y,\bar{z}$ (12) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				$hh\overline{2h}l$: $l=2n$ $000l$: $l=2n$
									Special: as above, plus
6	h	m . .	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$y,x,\frac{3}{4}$	$x-y,\bar{y},\frac{3}{4}$	$\bar{x},\bar{x}+y,\frac{3}{4}$	no extra conditions
6	g	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$hkil$: $l=2n$
4	f	3 . .	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	3 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
2	d	$\bar{6}$ . .	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	b	$\bar{6}$ . .	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	3 2 .	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

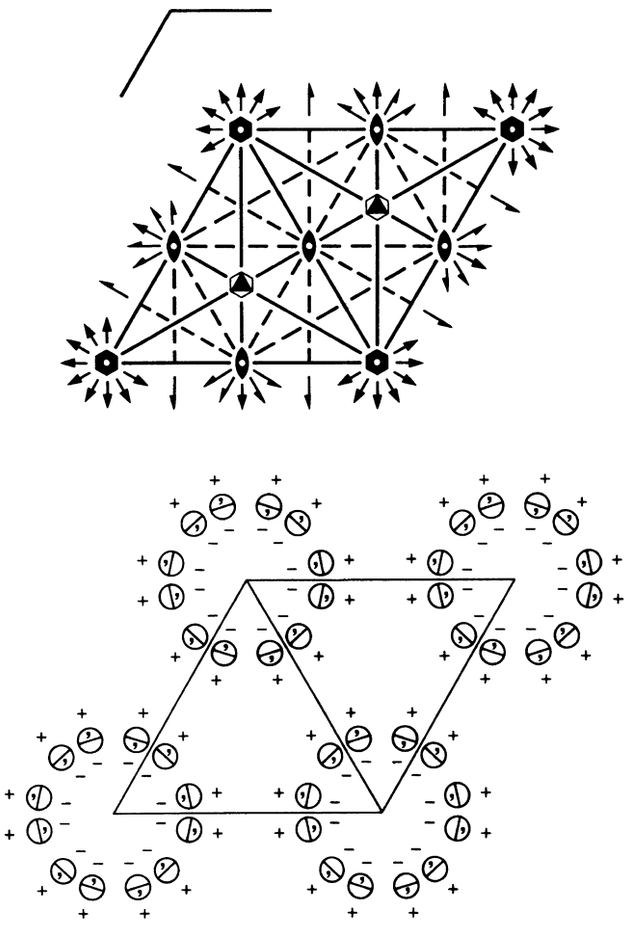
Along [001] $p3\,1m$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p1\,1m$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P6/mmm$ D_{6h}^{1} $6/mmm$ Hexagonal

No. 191 $P\ 6/m\ 2/m\ 2/m$ Patterson symmetry $P6/mmm$



Origin at centre $(6/mmm)$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{3}$; $0 \le z \le \frac{1}{2}$; $x \le (1+y)/2$; $y \le x/2$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$
$0,0,\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 3^+ $0,0,z$	(3) 3^- $0,0,z$
(4) 2 $0,0,z$	(5) 6^- $0,0,z$	(6) 6^+ $0,0,z$
(7) 2 $x,x,0$	(8) 2 $x,0,0$	(9) 2 $0,y,0$
(10) 2 $x,\bar{x},0$	(11) 2 $x,2x,0$	(12) 2 $2x,x,0$
(13) $\bar{1}$ $0,0,0$	(14) $\bar{3}^+$ $0,0,z$; $0,0,0$	(15) $\bar{3}^-$ $0,0,z$; $0,0,0$
(16) m $x,y,0$	(17) $\bar{6}^-$ $0,0,z$; $0,0,0$	(18) $\bar{6}^+$ $0,0,z$; $0,0,0$
(19) m $x,\bar{x},z$	(20) m $x,2x,z$	(21) m $2x,x,z$
(22) m x,x,z	(23) m $x,0,z$	(24) m $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
24	r	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}$ (10) $\bar{y},\bar{x},\bar{z}$ (13) $\bar{x},\bar{y},\bar{z}$ (16) $x,y,\bar{z}$ (19) $\bar{y},\bar{x},z$ (22) y,x,z	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $x-y,\bar{y},\bar{z}$ (11) $\bar{x}+y,y,\bar{z}$ (14) $y,\bar{x}+y,\bar{z}$ (17) $\bar{y},x-y,\bar{z}$ (20) $\bar{x}+y,y,z$ (23) $x-y,\bar{y},z$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $\bar{x},\bar{x}+y,\bar{z}$ (12) $x,x-y,\bar{z}$ (15) $x-y,x,\bar{z}$ (18) $\bar{x}+y,\bar{x},\bar{z}$ (21) $x,x-y,z$ (24) $\bar{x},\bar{x}+y,z$	no conditions
						Special: no extra conditions
12	q	m . .	$x,y,\frac{1}{2}$ $y,x,\frac{1}{2}$	$\bar{y},x-y,\frac{1}{2}$ $x-y,\bar{y},\frac{1}{2}$	$\bar{x}+y,\bar{x},\frac{1}{2}$ $\bar{x},\bar{x}+y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$ $\bar{y},\bar{x},\frac{1}{2}$	$y,\bar{x}+y,\frac{1}{2}$ $\bar{x}+y,y,\frac{1}{2}$	$x-y,x,\frac{1}{2}$ $x,x-y,\frac{1}{2}$
12	p	m . .	$x,y,0$ $y,x,0$	$\bar{y},x-y,0$ $x-y,\bar{y},0$	$\bar{x}+y,\bar{x},0$ $\bar{x},\bar{x}+y,0$	$\bar{x},\bar{y},0$ $\bar{y},\bar{x},0$	$y,\bar{x}+y,0$ $\bar{x}+y,y,0$	$x-y,x,0$ $x,x-y,0$
12	o	. m .	$x,2x,z$ $2x,x,\bar{z}$	$2\bar{x},\bar{x},z$ $\bar{x},2\bar{x},\bar{z}$	$x,\bar{x},z$ $\bar{x},x,\bar{z}$	$\bar{x},2\bar{x},z$ $2\bar{x},\bar{x},\bar{z}$	$2x,x,z$ $x,2x,\bar{z}$	$\bar{x},x,z$ $x,\bar{x},\bar{z}$
12	n	. . m	$x,0,z$ $0,x,\bar{z}$	$0,x,z$ $x,0,\bar{z}$	$\bar{x},\bar{x},z$ $\bar{x},\bar{x},\bar{z}$	$\bar{x},0,z$ $0,\bar{x},\bar{z}$	$0,\bar{x},z$ $\bar{x},0,\bar{z}$	x,x,z $x,x,\bar{z}$
6	m	$m\,m\,2$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$
6	l	$m\,m\,2$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},2\bar{x},0$	$2x,x,0$	$\bar{x},x,0$
6	k	$m\,2\,m$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$
6	j	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$
6	i	$2\,m\,m$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$	$\frac{1}{2},\frac{1}{2},\bar{z}$
4	h	$3\,m$.	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}$		
3	g	$m\,m\,m$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
3	f	$m\,m\,m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2	e	$6\,m\,m$	$0,0,z$	$0,0,\bar{z}$				
2	d	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$				
2	c	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$				
1	b	$6/m\,m\,m$	$0,0,\frac{1}{2}$					
1	a	$6/m\,m\,m$	$0,0,0$					

Symmetry of special projections

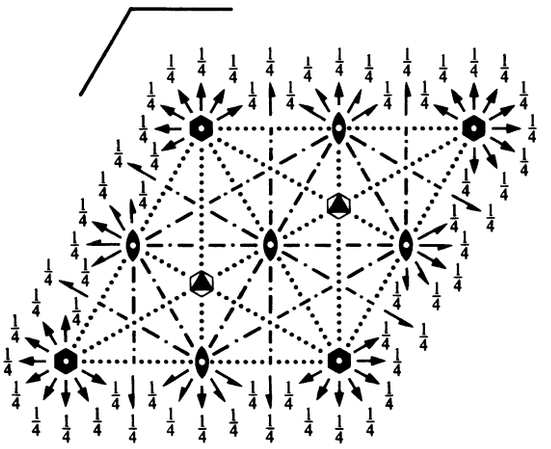
Along [001] $p6mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

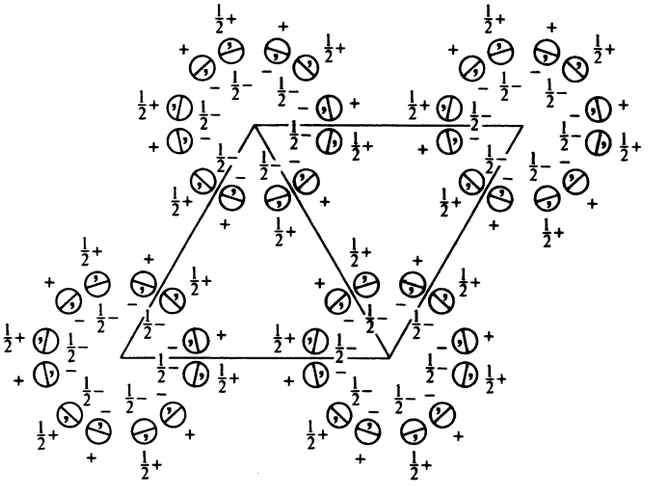
Along [100] $p2mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P6/mcc$ D_{6h}^2 $6/mmm$ Hexagonal

No. 192 $P\ 6/m\ 2/c\ 2/c$ Patterson symmetry $P6/mmm$





Origin at centre $(6/m)$ at $6/mcc$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{2},\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) 2 $0,0,z$
(5) 6^- $0,0,z$
(6) 6^+ $0,0,z$
(7) 2 $x,x,\frac{1}{4}$
(8) 2 $x,0,\frac{1}{4}$
(9) 2 $0,y,\frac{1}{4}$
(10) 2 $x,\bar{x},\frac{1}{4}$
(11) 2 $x,2x,\frac{1}{4}$
(12) 2 $2x,x,\frac{1}{4}$
(13) $\bar{1}$ $0,0,0$
(14) $\bar{3}^+$ $0,0,z$; $0,0,0$
(15) $\bar{3}^-$ $0,0,z$; $0,0,0$
(16) m $x,y,0$
(17) $\bar{6}^-$ $0,0,z$; $0,0,0$
(18) $\bar{6}^+$ $0,0,z$; $0,0,0$
(19) c $x,\bar{x},z$
(20) c $x,2x,z$
(21) c $2x,x,z$
(22) c x,x,z
(23) c $x,0,z$
(24) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
24	m	1	(1) x,y,z (4) $\bar{x},\bar{y},z$ (7) $y,x,\bar{z}+\frac{1}{2}$ (10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$ (13) $\bar{x},\bar{y},\bar{z}$ (16) $x,y,\bar{z}$ (19) $\bar{y},\bar{x},z+\frac{1}{2}$ (22) $y,x,z+\frac{1}{2}$	(2) $\bar{y},x-y,z$ (5) $y,\bar{x}+y,z$ (8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$ (11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$ (14) $y,\bar{x}+y,\bar{z}$ (17) $\bar{y},x-y,\bar{z}$ (20) $\bar{x}+y,y,z+\frac{1}{2}$ (23) $x-y,\bar{y},z+\frac{1}{2}$	(3) $\bar{x}+y,\bar{x},z$ (6) $x-y,x,z$ (9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$ (12) $x,x-y,\bar{z}+\frac{1}{2}$ (15) $x-y,x,\bar{z}$ (18) $\bar{x}+y,\bar{x},\bar{z}$ (21) $x,x-y,z+\frac{1}{2}$ (24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				$hh\overline{2h}l$: $l=2n$ $h\bar{h}0l$: $l=2n$ $000l$: $l=2n$
									Special: as above, plus
12	l	m . .	$x,y,0$ $y,x,\frac{1}{2}$	$\bar{y},x-y,0$ $x-y,\bar{y},\frac{1}{2}$	$\bar{x}+y,\bar{x},0$ $\bar{x},\bar{x}+y,\frac{1}{2}$	$\bar{x},\bar{y},0$ $\bar{y},\bar{x},\frac{1}{2}$	$y,\bar{x}+y,0$ $\bar{x}+y,y,\frac{1}{2}$	$x-y,x,0$ $x,x-y,\frac{1}{2}$	no extra conditions
12	k	. . 2	$x,2x,\frac{1}{4}$ $\bar{x},2\bar{x},\frac{3}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$ $2x,x,\frac{3}{4}$	$x,\bar{x},\frac{1}{4}$ $\bar{x},x,\frac{3}{4}$	$\bar{x},2\bar{x},\frac{1}{4}$ $x,2x,\frac{3}{4}$	$2x,x,\frac{1}{4}$ $2\bar{x},\bar{x},\frac{3}{4}$	$\bar{x},x,\frac{1}{4}$ $x,\bar{x},\frac{3}{4}$	$hkil$: $l=2n$
12	j	. 2 .	$x,0,\frac{1}{4}$ $\bar{x},0,\frac{3}{4}$	$0,x,\frac{1}{4}$ $0,\bar{x},\frac{3}{4}$	$\bar{x},\bar{x},\frac{1}{4}$ $x,x,\frac{3}{4}$	$\bar{x},0,\frac{1}{4}$ $x,0,\frac{3}{4}$	$0,\bar{x},\frac{1}{4}$ $0,x,\frac{3}{4}$	$x,x,\frac{1}{4}$ $\bar{x},\bar{x},\frac{3}{4}$	$hkil$: $l=2n$
12	i	2 . .	$\frac{1}{2},0,z$ $\frac{1}{2},0,\bar{z}$	$0,\frac{1}{2},z$ $0,\frac{1}{2},\bar{z}$	$\frac{1}{2},\frac{1}{2},z$ $\frac{1}{2},\frac{1}{2},\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$hkil$: $l=2n$
8	h	3 . .	$\frac{1}{3},\frac{2}{3},z$ $\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},z$ $\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$			$hkil$: $l=2n$
6	g	$2/m$ . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
6	f	2 2 2	$\frac{1}{2},0,\frac{1}{4}$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	$hkil$: $l=2n$
4	e	6 . .	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$			$hkil$: $l=2n$
4	d	$\bar{6}$ . .	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			$hkil$: $l=2n$
4	c	3 . 2	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$			$hkil$: $l=2n$
2	b	$6/m$ . .	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	6 2 2	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

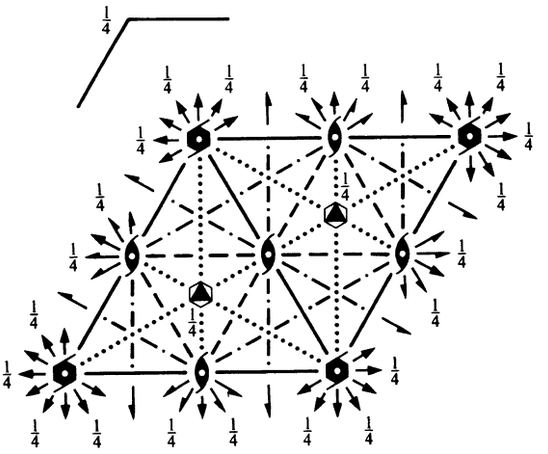
Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

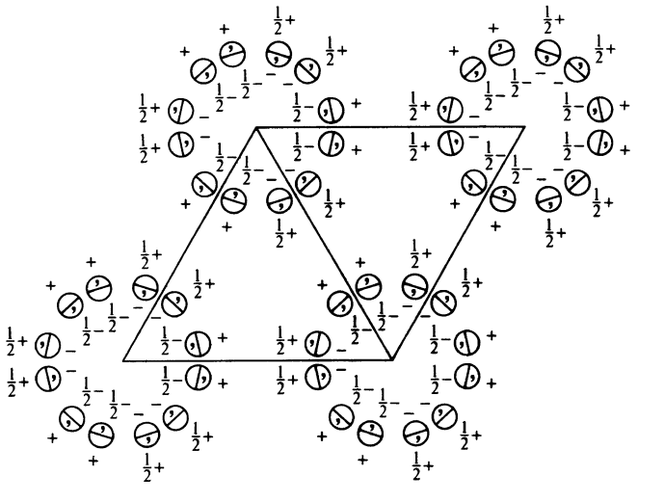
Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P6_3/mcm$ D_{6h}^3 $6/mmm$ Hexagonal

No. 193 $P\ 6_3/m\ 2/c\ 2/m$ Patterson symmetry $P6/mmm$



For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)



Origin at centre $(\bar{3}\,1\,m)$ at $\bar{3}\,c\,2/m$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $x \le (1+y)/2$; $y \le \min(1-x,x)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{2},\frac{1}{2},0$
$0,0,\frac{1}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{2},\frac{1}{2},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$
(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$
(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) 2 $x,x,\frac{1}{4}$
(8) 2 $x,0,\frac{1}{4}$
(9) 2 $0,y,\frac{1}{4}$
(10) 2 $x,\bar{x},0$
(11) 2 $x,2x,0$
(12) 2 $2x,x,0$
(13) $\bar{1}$ $0,0,0$
(14) $\bar{3}^+$ $0,0,z$; $0,0,0$
(15) $\bar{3}^-$ $0,0,z$; $0,0,0$
(16) m $x,y,\frac{1}{4}$
(17) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$
(18) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(19) c $x,\bar{x},z$
(20) c $x,2x,z$
(21) c $2x,x,z$
(22) m x,x,z
(23) m $x,0,z$
(24) m $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$h\bar{h}0l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				$000l$: $l=2n$
			(7) $y,x,\bar{z}+\frac{1}{2}$	(8) $x-y,\bar{y},\bar{z}+\frac{1}{2}$	(9) $\bar{x},\bar{x}+y,\bar{z}+\frac{1}{2}$				
			(10) $\bar{y},\bar{x},\bar{z}$	(11) $\bar{x}+y,y,\bar{z}$	(12) $x,x-y,\bar{z}$				
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$				
			(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				
			(19) $\bar{y},\bar{x},z+\frac{1}{2}$	(20) $\bar{x}+y,y,z+\frac{1}{2}$	(21) $x,x-y,z+\frac{1}{2}$				
			(22) y,x,z	(23) $x-y,\bar{y},z$	(24) $\bar{x},\bar{x}+y,z$				
									Special: as above, plus
12	k	$..m$	$x,0,z$	$0,x,z$	$\bar{x},\bar{x},z$	$\bar{x},0,z+\frac{1}{2}$			no extra conditions
			$0,\bar{x},z+\frac{1}{2}$	$x,x,z+\frac{1}{2}$	$0,x,\bar{z}+\frac{1}{2}$	$x,0,\bar{z}+\frac{1}{2}$			
			$\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$0,\bar{x},\bar{z}$	$\bar{x},0,\bar{z}$	$x,x,\bar{z}$			
12	j	$m..$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
			$y,x,\frac{1}{4}$	$x-y,\bar{y},\frac{1}{4}$	$\bar{x},\bar{x}+y,\frac{1}{4}$	$\bar{y},\bar{x},\frac{3}{4}$	$\bar{x}+y,y,\frac{3}{4}$	$x,x-y,\frac{3}{4}$	
12	i	$..2$	$x,2x,0$	$2\bar{x},\bar{x},0$	$x,\bar{x},0$	$\bar{x},2\bar{x},\frac{1}{2}$	$2x,x,\frac{1}{2}$	$\bar{x},x,\frac{1}{2}$	$hkil$: $l=2n$
			$\bar{x},2\bar{x},0$	$2x,x,0$	$\bar{x},x,0$	$x,2x,\frac{1}{2}$	$2\bar{x},\bar{x},\frac{1}{2}$	$x,\bar{x},\frac{1}{2}$	
8	h	$3..$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},\bar{z}$			$hkil$: $l=2n$
			$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$	$\frac{1}{3},\frac{2}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},z$			
6	g	$m\,2\,m$	$x,0,\frac{1}{4}$	$0,x,\frac{1}{4}$	$\bar{x},\bar{x},\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$0,\bar{x},\frac{3}{4}$	$x,x,\frac{3}{4}$	no extra conditions
6	f	$..2/m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	e	$3\,.\,m$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$			$hkil$: $l=2n$
4	d	$3\,.\,2$	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},0$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$			$hkil$: $l=2n$
4	c	$\bar{6}..$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$			$hkil$: $l=2n$
2	b	$\bar{3}\,.\,m$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$
2	a	$\bar{6}\,2\,m$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$

Symmetry of special projections

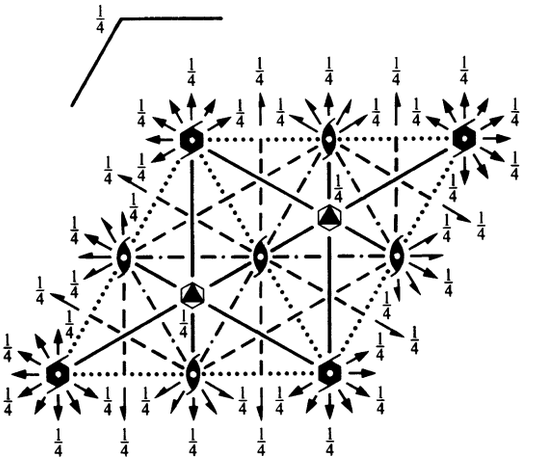
Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,0,0$

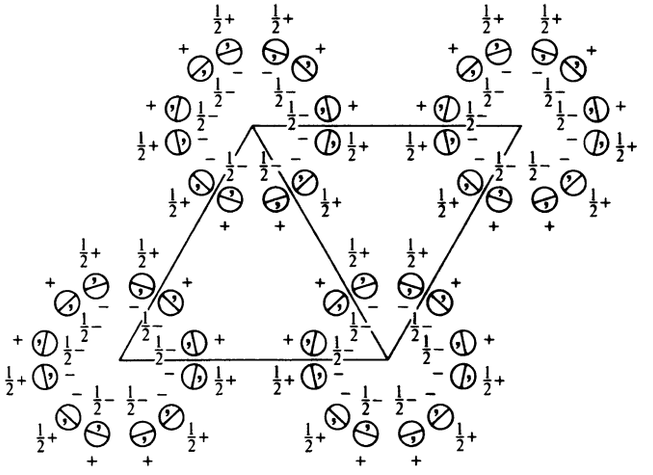
Along [210] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P6_3/mmc$ D_{6h}^4 $6/mmm$ Hexagonal

No. 194 $P\ 6_3/m\ 2/m\ 2/c$ Patterson symmetry $P6/mmm$



For $\bar{1}$ and $\bar{6}$ see $P6_3/m$ (No. 176)



Origin at centre $(\bar{3}m1)$ at $\bar{3}2/mc$

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $0 \le z \le \frac{1}{4}$; $x \le 2y$; $y \le \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$
$0,0,\frac{1}{4}$ $\frac{2}{3},\frac{1}{3},\frac{1}{4}$ $\frac{1}{3},\frac{2}{3},\frac{1}{4}$

Symmetry operations

(1) 1
(2) 3^+ $0,0,z$
(3) 3^- $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$
(5) $6^-(0,0,\frac{1}{2})$ $0,0,z$
(6) $6^+(0,0,\frac{1}{2})$ $0,0,z$
(7) 2 $x,x,0$
(8) 2 $x,0,0$
(9) 2 $0,y,0$
(10) 2 $x,\bar{x},\frac{1}{4}$
(11) 2 $x,2x,\frac{1}{4}$
(12) 2 $2x,x,\frac{1}{4}$
(13) $\bar{1}$ $0,0,0$
(14) $\bar{3}^+$ $0,0,z$; $0,0,0$
(15) $\bar{3}^-$ $0,0,z$; $0,0,0$
(16) m $x,y,\frac{1}{4}$
(17) $\bar{6}^-$ $0,0,z$; $0,0,\frac{1}{4}$
(18) $\bar{6}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(19) m $x,\bar{x},z$
(20) m $x,2x,z$
(21) m $2x,x,z$
(22) c x,x,z
(23) c $x,0,z$
(24) c $0,y,z$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4); (7); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									General:
24	l	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$				$hh\overline{2h}l$: $l=2n$ $000l$: $l=2n$
			(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{1}{2}$	(6) $x-y,x,z+\frac{1}{2}$				
			(7) $y,x,\bar{z}$	(8) $x-y,\bar{y},\bar{z}$	(9) $\bar{x},\bar{x}+y,\bar{z}$				
			(10) $\bar{y},\bar{x},\bar{z}+\frac{1}{2}$	(11) $\bar{x}+y,y,\bar{z}+\frac{1}{2}$	(12) $x,x-y,\bar{z}+\frac{1}{2}$				
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $y,\bar{x}+y,\bar{z}$	(15) $x-y,x,\bar{z}$				
			(16) $x,y,\bar{z}+\frac{1}{2}$	(17) $\bar{y},x-y,\bar{z}+\frac{1}{2}$	(18) $\bar{x}+y,\bar{x},\bar{z}+\frac{1}{2}$				
			(19) $\bar{y},\bar{x},z$	(20) $\bar{x}+y,y,z$	(21) $x,x-y,z$				
			(22) $y,x,z+\frac{1}{2}$	(23) $x-y,\bar{y},z+\frac{1}{2}$	(24) $\bar{x},\bar{x}+y,z+\frac{1}{2}$				
									Special: as above, plus
12	k	$.m.$	$x,2x,z$	$2\bar{x},\bar{x},z$	$x,\bar{x},z$	$\bar{x},2\bar{x},z+\frac{1}{2}$			no extra conditions
			$2x,x,z+\frac{1}{2}$	$\bar{x},x,z+\frac{1}{2}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$			
			$\bar{x},x,\bar{z}$	$2\bar{x},\bar{x},\bar{z}+\frac{1}{2}$	$x,2x,\bar{z}+\frac{1}{2}$	$x,\bar{x},\bar{z}+\frac{1}{2}$			
12	j	$m..$	$x,y,\frac{1}{4}$	$\bar{y},x-y,\frac{1}{4}$	$\bar{x}+y,\bar{x},\frac{1}{4}$	$\bar{x},\bar{y},\frac{3}{4}$	$y,\bar{x}+y,\frac{3}{4}$	$x-y,x,\frac{3}{4}$	no extra conditions
			$y,x,\frac{3}{4}$	$x-y,\bar{y},\frac{3}{4}$	$\bar{x},\bar{x}+y,\frac{3}{4}$	$\bar{y},\bar{x},\frac{1}{4}$	$\bar{x}+y,y,\frac{1}{4}$	$x,x-y,\frac{1}{4}$	
12	i	$.2.$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$	$hkil$: $l=2n$
			$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	
6	h	$m\,m\,2$	$x,2x,\frac{1}{4}$	$2\bar{x},\bar{x},\frac{1}{4}$	$x,\bar{x},\frac{1}{4}$	$\bar{x},2\bar{x},\frac{3}{4}$	$2x,x,\frac{3}{4}$	$\bar{x},x,\frac{3}{4}$	no extra conditions
6	g	$.2/m.$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$hkil$: $l=2n$
4	f	$3\,m.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},z+\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\bar{z}$	$\frac{1}{3},\frac{2}{3},\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
4	e	$3\,m.$	$0,0,z$	$0,0,z+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,\bar{z}+\frac{1}{2}$			$hkil$: $l=2n$
2	d	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},\frac{3}{4}$	$\frac{2}{3},\frac{1}{3},\frac{1}{4}$					$hkil$: $l=2n$ or $h-k=3n+1$ or $h-k=3n+2$
2	c	$\bar{6}\,m\,2$	$\frac{1}{3},\frac{2}{3},\frac{1}{4}$	$\frac{2}{3},\frac{1}{3},\frac{3}{4}$					
2	b	$\bar{6}\,m\,2$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$					$hkil$: $l=2n$
2	a	$\bar{3}\,m.$	$0,0,0$	$0,0,\frac{1}{2}$					$hkil$: $l=2n$

Symmetry of special projections

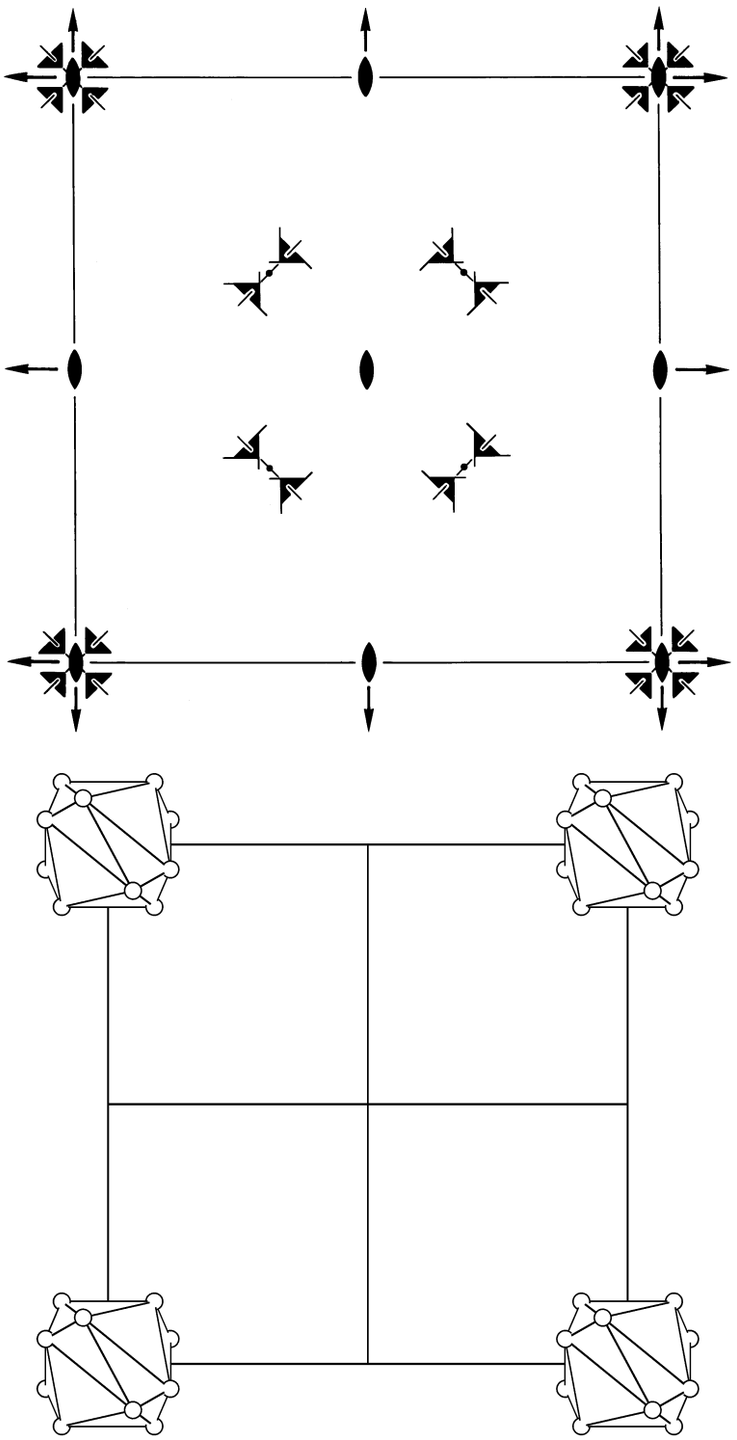
Along [001] $p6mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}+2\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [210] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,\frac{1}{2}x,0$

$P23$ T^1 23 Cubic

No. 195 $P23$ Patterson symmetry $Pm\bar{3}$



Origin at 23

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le 1;\quad 0 \le z \le \frac{1}{2};\quad y \le 1-x;\quad z \le \min(x,y)$

Vertices $0,0,0\quad 1,0,0\quad 0,1,0\quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l cyclically permutable
									General:
12	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
									Special: no extra conditions
6	i	2 . .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	
6	h	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
6	g	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	
6	f	2 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
4	e	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
3	d	2 2 2 . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
3	c	2 2 2 . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
1	b	2 3 .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	2 3 .	$0,0,0$						

Symmetry of special projections

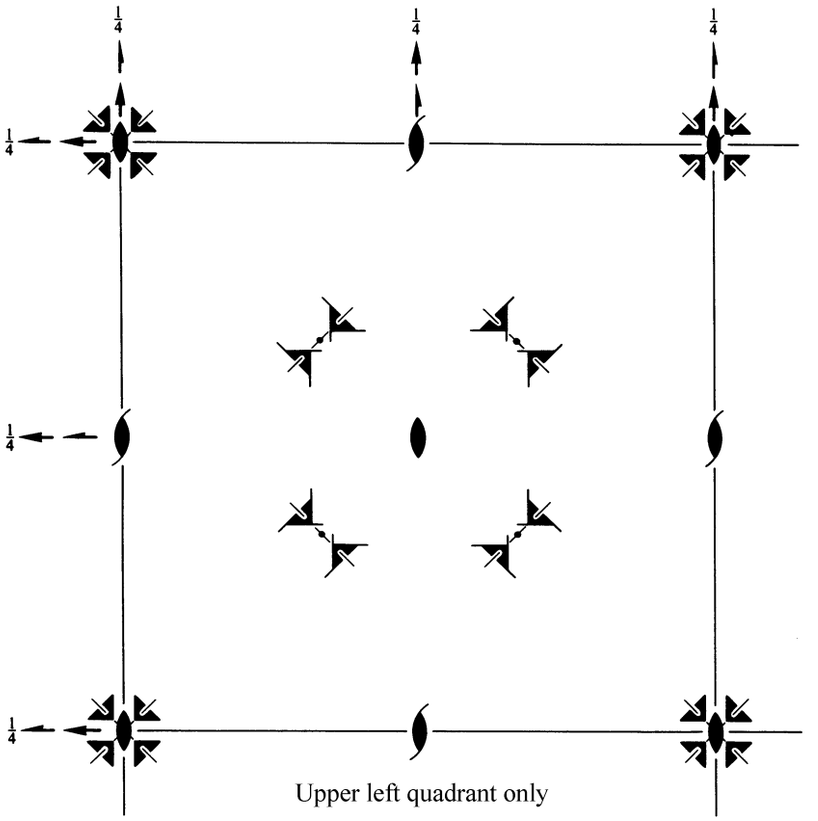
Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

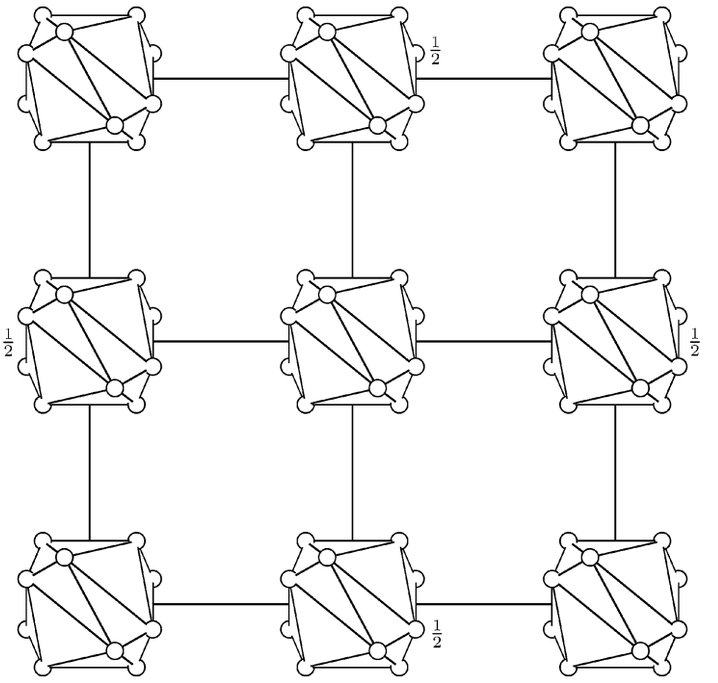
Along [111] $p3$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$F\,2\,3$ T^2 2 3 Cubic

No. 196 $F\,2\,3$ Patterson symmetry $F\,m\,\bar{3}$





Origin at 2 3

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le x$; $\max(x-\frac{1}{2},-y) \le z \le \min(\frac{1}{2}-x,y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2\quad 0,0,z$	(3) $2\quad 0,y,0$	(4) $2\quad x,0,0$
(5) $3^+\ x,x,x$	(6) $3^+\ \bar{x},x,\bar{x}$	(7) $3^+\ x,\bar{x},\bar{x}$	(8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-\ x,x,x$	(10) $3^-\ x,\bar{x},\bar{x}$	(11) $3^-\ \bar{x},\bar{x},x$	(12) $3^-\ \bar{x},x,\bar{x}$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$	(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$	(6) $3^+\ \bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^+\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) $3^-\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$	(3) $2\quad \frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) $3^+\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^+\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^-\ x+\frac{1}{2},\bar{x},\bar{x}$	(11) $3^-\ \bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2\quad \frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^+\ \bar{x}+\frac{1}{2},x,\bar{x}$	(7) $3^+\ x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^-\ x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-\ \bar{x},x+\frac{1}{2},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$		Reflection conditions
								h,k,l cyclically permutable General:
48	h	1	(1) x,y,z (5) z,x,y (9) y,z,x	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$		hkl: $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ hhl: $h+l=2n$ $h00$: $h=2n$
								Special: no extra conditions
24	g	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$
24	f	2 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
16	e	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
4	d	2 3 .	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					
4	c	2 3 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$					
4	b	2 3 .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
4	a	2 3 .	$0,0,0$					

Symmetry of special projections

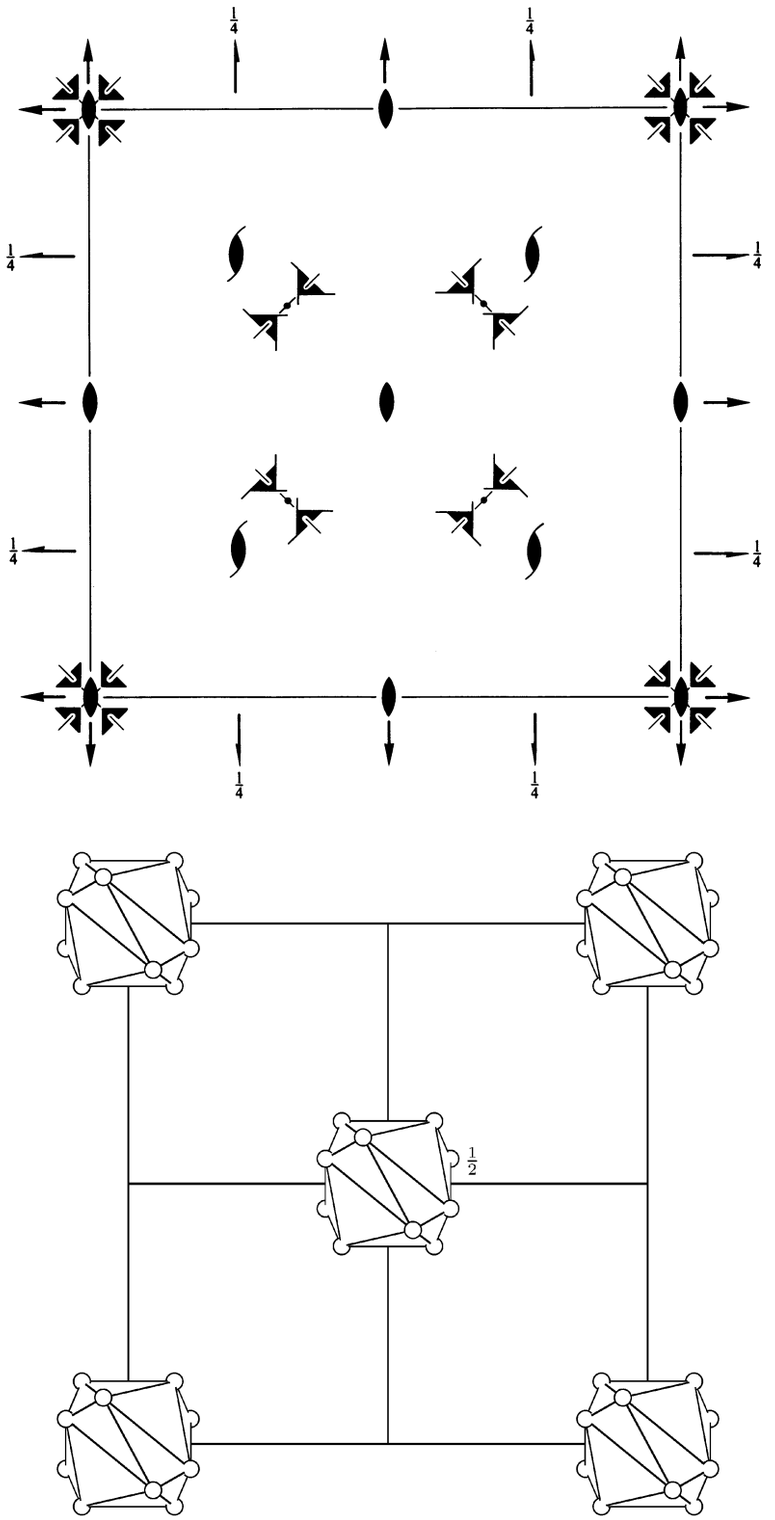
Along [001] $p\,2\,m\,m$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}\qquad \mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p\,3$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})\qquad \mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\qquad \mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$I23$ T^3 23 Cubic

No. 197 $I23$ Patterson symmetry $Im\bar{3}$



Origin at 23

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad y \le \min(x, 1-x); \quad z \le y$

Vertices $0,0,0 \quad 1,0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$					Reflection conditions
									h,k,l cyclically permutable
									General:
24	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $h00$: $h=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
									Special: no extra conditions
12	e	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
12	d	2 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
8	c	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
6	b	2 2 2 . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
2	a	2 3 .	$0,0,0$						

Symmetry of special projections

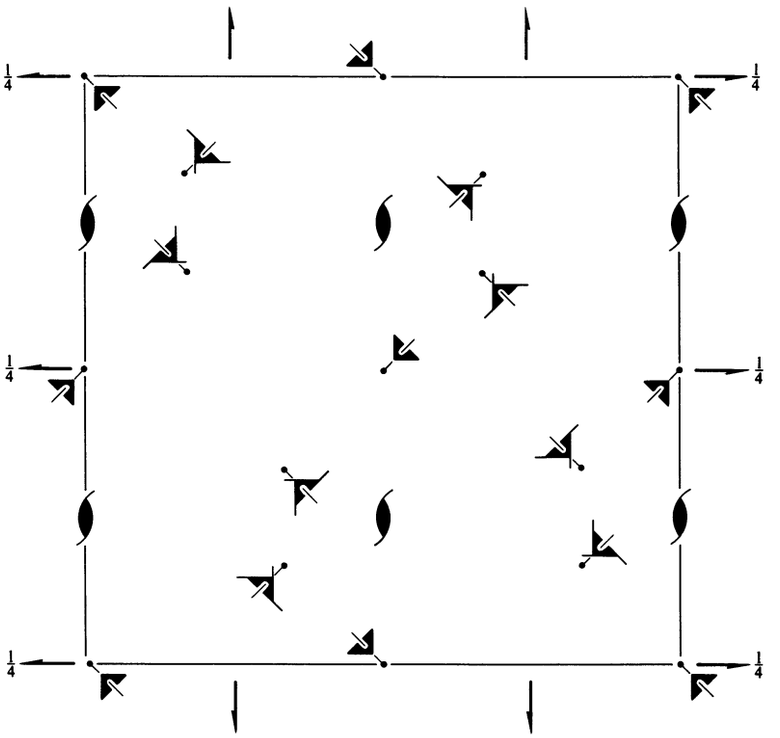
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

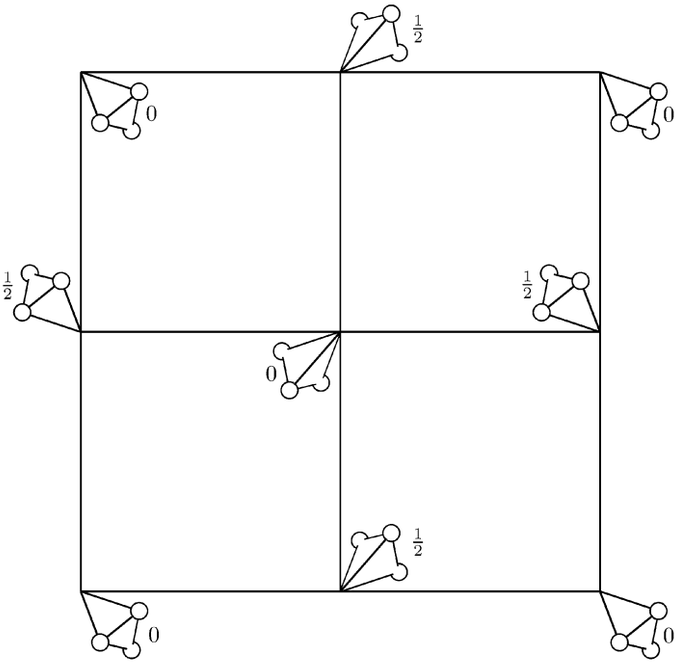
Along [111] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P2_13$ T^4 23 Cubic

No. 198 $P2_13$ Patterson symmetry $Pm\bar{3}$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $-\frac{1}{2} \le z \le \frac{1}{2}$; $\max(x-\frac{1}{2}, -y) \le z \le \min(x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $0,\frac{1}{2},-\frac{1}{2}$

Symmetry operations

(1) 1
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

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Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					h,k,l cyclically permutable
					General:
12 b 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00$: $h=2n$
	(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	
	(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
					Special: no extra conditions
4 a . 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	

Symmetry of special projections

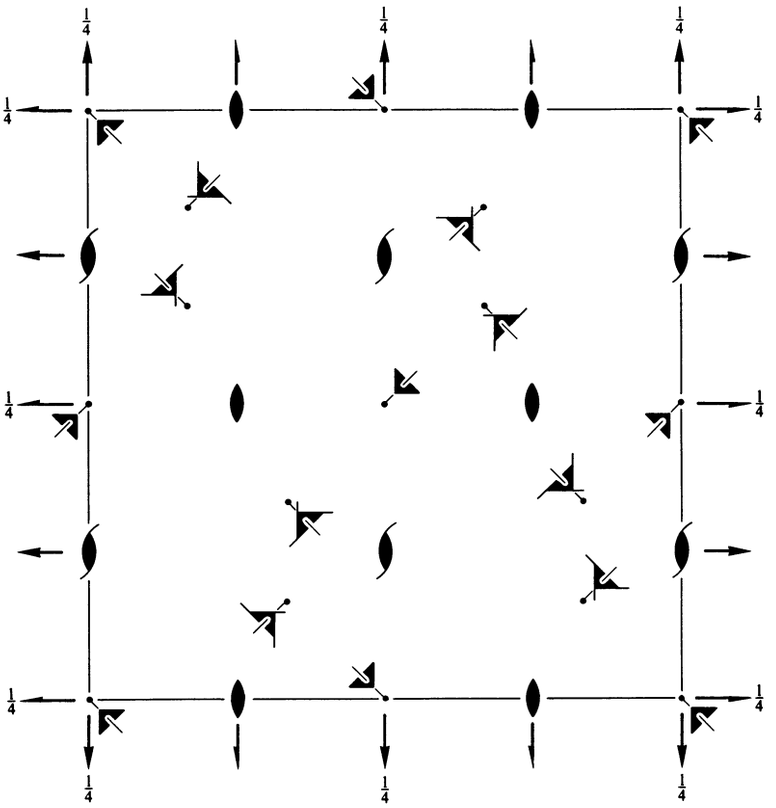
Along [001] $p2gg$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

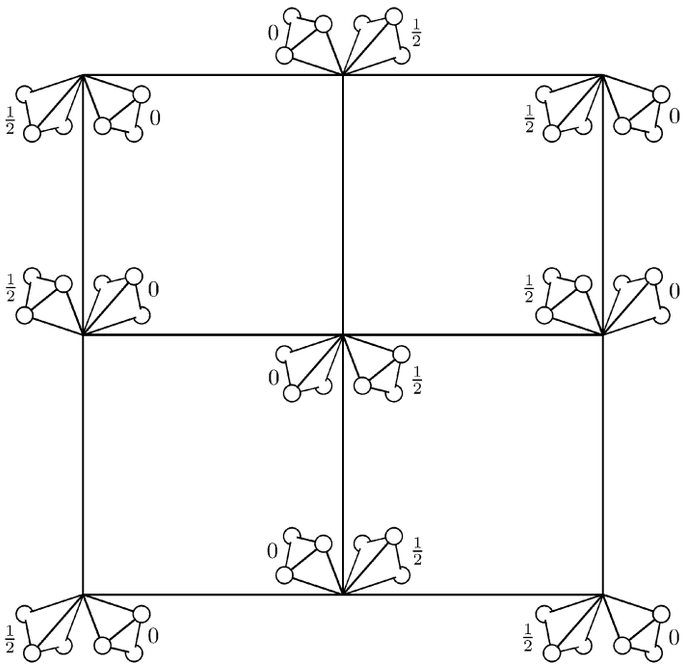
Along [111] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1g1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x+\frac{1}{4},x,0$

$I2_13$ T^5 23 Cubic

No. 199 $I2_13$ Patterson symmetry $Im\bar{3}$





Origin on 3[111] at midpoint of three non-intersecting pairs of parallel 2 axes and of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,0$	(4) 2 $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							h,k,l cyclically permutable
							General:
24	c	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	hhl: $l=2n$
							$h00$: $h=2n$
							Special: no extra conditions
12	b	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$ $0,\frac{3}{4},\bar{x}+\frac{1}{2}$
8	a	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	

Symmetry of special projections

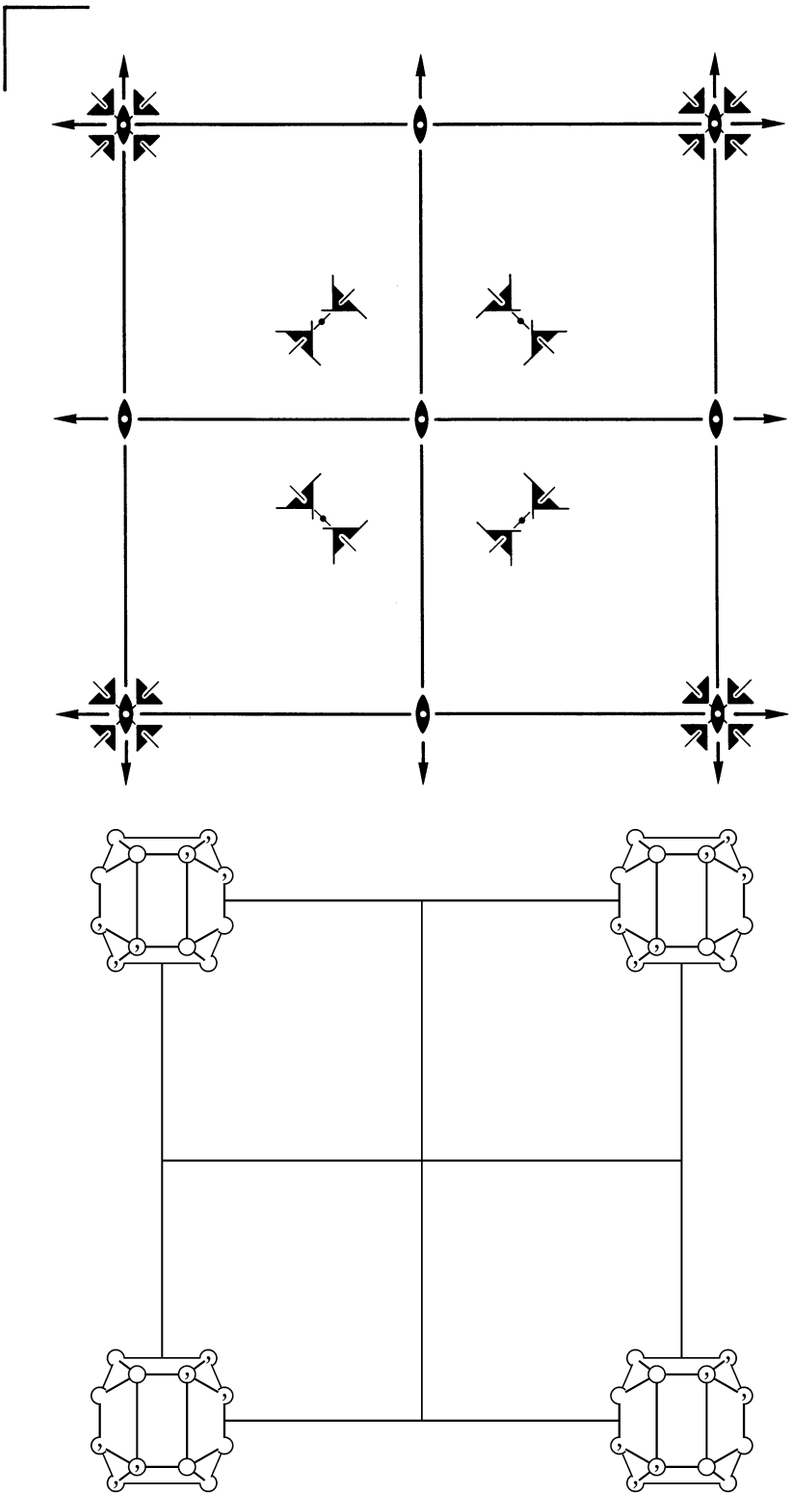
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [111] $p3$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},0$

$Pm\bar{3}$ T_h^1 $m\bar{3}$ Cubic

No. 200 $P2/m\bar{3}$ Patterson symmetry $Pm\bar{3}$



Origin at centre $(m\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x,y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $\bar{1}$ $0,0,0$	(14) m $x,y,0$	(15) m $x,0,z$	(16) m $0,y,z$
(17) $\bar{3}^+$ $x,x,x;$ $0,0,0$	(18) $\bar{3}^+$ $\bar{x},x,\bar{x};$ $0,0,0$	(19) $\bar{3}^+$ $x,\bar{x},\bar{x};$ $0,0,0$	(20) $\bar{3}^+$ $\bar{x},\bar{x},x;$ $0,0,0$
(21) $\bar{3}^-$ $x,x,x;$ $0,0,0$	(22) $\bar{3}^-$ $x,\bar{x},\bar{x};$ $0,0,0$	(23) $\bar{3}^-$ $\bar{x},\bar{x},x;$ $0,0,0$	(24) $\bar{3}^-$ $\bar{x},x,\bar{x};$ $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l cyclically permutable
									General:
24	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$			
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$			
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$			
									Special: no extra conditions
12	k	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$z,\frac{1}{2},y$	$z,\frac{1}{2},\bar{y}$	
			$\bar{z},\frac{1}{2},y$	$\bar{z},\frac{1}{2},\bar{y}$	$y,z,\frac{1}{2}$	$\bar{y},z,\frac{1}{2}$	$y,\bar{z},\frac{1}{2}$	$\bar{y},\bar{z},\frac{1}{2}$	
12	j	m . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$	
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	
8	i	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
			$\bar{x},\bar{x},\bar{x}$	$x,x,\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
6	h	$m\,m\,2$ . .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	
6	g	$m\,m\,2$ . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
6	f	$m\,m\,2$ . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	
6	e	$m\,m\,2$ . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
3	d	$m\,m\,m$ . .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
3	c	$m\,m\,m$ . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
1	b	$m\,\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	$m\,\bar{3}$.	$0,0,0$						

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

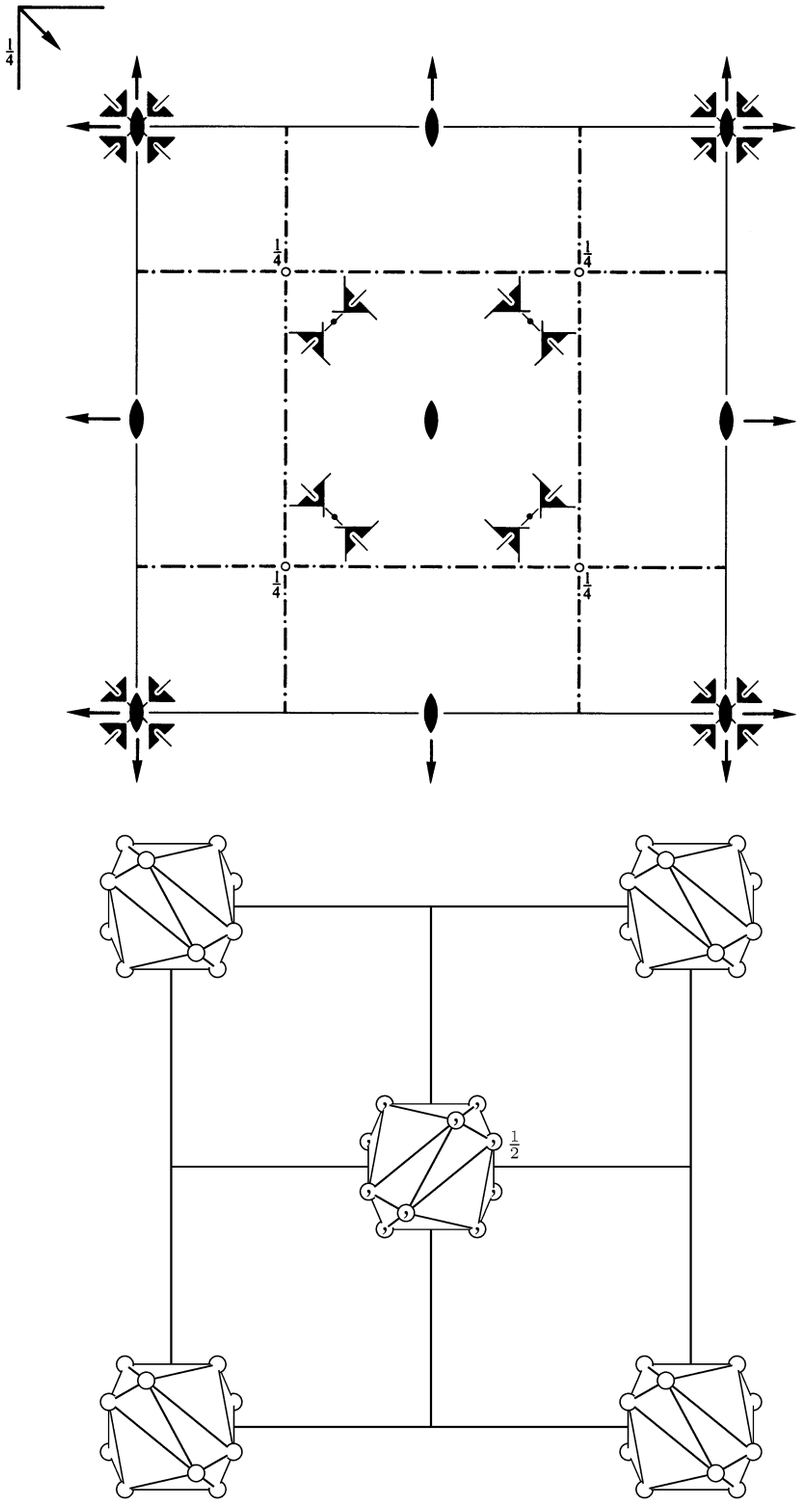
Along [111] $p6$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$Pn\bar{3}$ T_h^2 $m\bar{3}$ Cubic

No. 201 $P2/n\bar{3}$ Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 1



Origin at 23, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre $(\bar{3})$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad y \le \min(x, 1-x);\quad z \le y$

Vertices $0,0,0\quad 1,0,0\quad \frac{1}{2},\frac{1}{2},0\quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}$,x,$\bar{x}$	(7) 3^+ x,$\bar{x}$,$\bar{x}$	(8) 3^+ $\bar{x}$,$\bar{x}$,x
(9) 3^- x,x,x	(10) 3^- x,$\bar{x}$,$\bar{x}$	(11) 3^- $\bar{x}$,$\bar{x}$,x	(12) 3^- $\bar{x}$,x,$\bar{x}$
(13) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(14) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(15) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(16) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(17) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(18) $\bar{3}^+$ $\bar{x}$−1,x+1,$\bar{x}$; $-\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(19) $\bar{3}^+$ x,$\bar{x}$+1,$\bar{x}$; $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+$ $\bar{x}$+1,$\bar{x}$,x; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(21) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(22) $\bar{3}^-$ x+1,$\bar{x}$−1,$\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^-$ $\bar{x}$,$\bar{x}$+1,x; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(24) $\bar{3}^-$ $\bar{x}$+1,x,$\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l cyclically permutable
									General:
24	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			$0kl$: $k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
			(13) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$			
			(17) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(19) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$			
			(21) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(24) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$			
									Special: as above, plus
12	g	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$x+\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	$0,\frac{1}{2},\bar{x}+\frac{1}{2}$	$0,\frac{1}{2},x+\frac{1}{2}$	
12	f	2 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	
8	e	. 3 .	x,x,x	$\bar{x},\bar{x},x$					no extra conditions
			$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$					
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$					
			$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
6	d	2 2 2 . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$	hkl: $h+k+l=2n$
4	c	. $\bar{3}$.	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl: $h+k,h+l,k+l=2n$
4	b	. $\bar{3}$.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k,h+l,k+l=2n$
2	a	2 3 .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl: $h+k+l=2n$

Symmetry of special projections

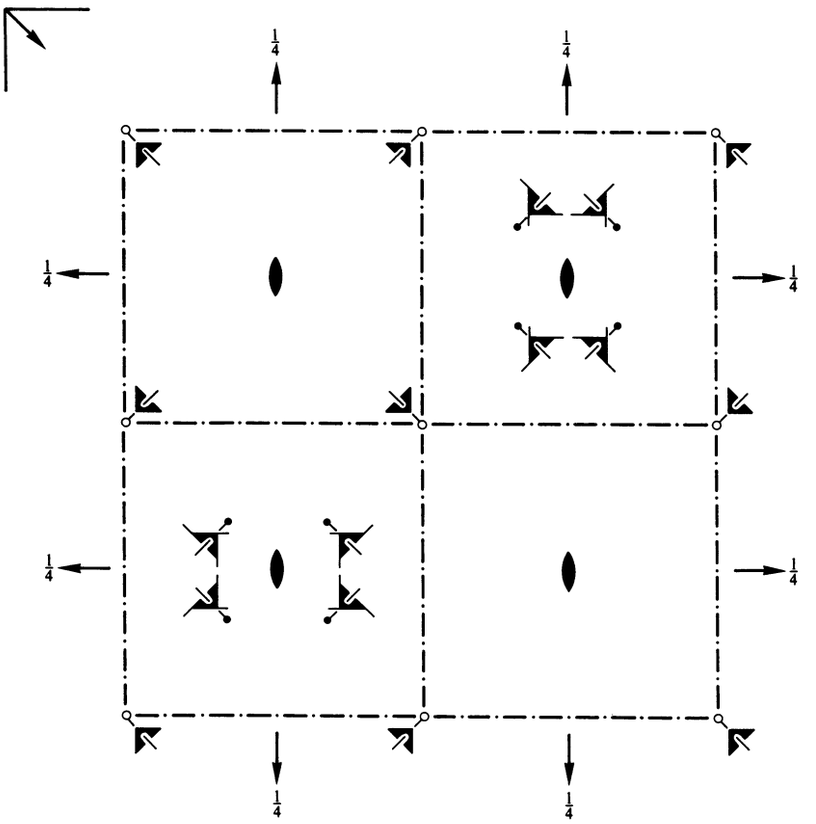
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

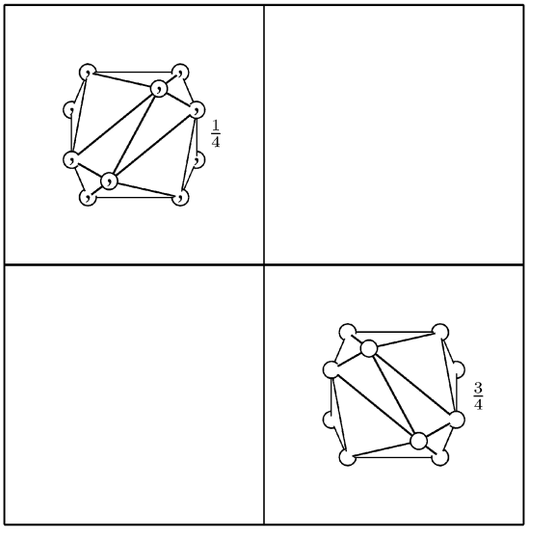
Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

No. 201 $P2/n\bar{3}$ Patterson symmetry $Pm\bar{3}$

ORIGIN CHOICE 2





Origin at centre $(\bar{3})$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 23

Asymmetric unit $-\frac{1}{4} \le x \le \frac{3}{4}$; $-\frac{1}{4} \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2}-x)$; $z \le y$

Vertices $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ $\frac{3}{4},-\frac{1}{4},-\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

(1) 1	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$	(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}$ 0,0,0	(14) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$	(15) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$	(16) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
(17) $\bar{3}^+$ x,x,x; 0,0,0	(18) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; $-\frac{1}{2},0,\frac{1}{2}$	(19) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+1,\bar{x}$; $0,\frac{1}{2},-\frac{1}{2}$	(20) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{1}{2},-\frac{1}{2},0$
(21) $\bar{3}^-$ x,x,x; 0,0,0	(22) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-1,\bar{x}$; $0,-\frac{1}{2},\frac{1}{2}$	(23) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; $-\frac{1}{2},\frac{1}{2},0$	(24) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,-\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l cyclically permutable
									General:
24	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$			$0kl$: $k+l=2n$
			(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$			$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$			
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(15) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(16) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$			
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(19) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(20) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$			
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(23) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(24) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$			
									Special: as above, plus
12	g	2 . .	$x,\frac{3}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl: $h+k+l=2n$
			$\bar{x},\frac{1}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{1}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x+\frac{1}{2}$	
12	f	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl: $h+k+l=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$	
8	e	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},x+\frac{1}{2}$			
6	d	2 2 2 . .	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h+k+l=2n$
4	c	. $\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k,h+l,k+l=2n$
4	b	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k,h+l,k+l=2n$
2	a	2 3 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl: $h+k+l=2n$

Symmetry of special projections

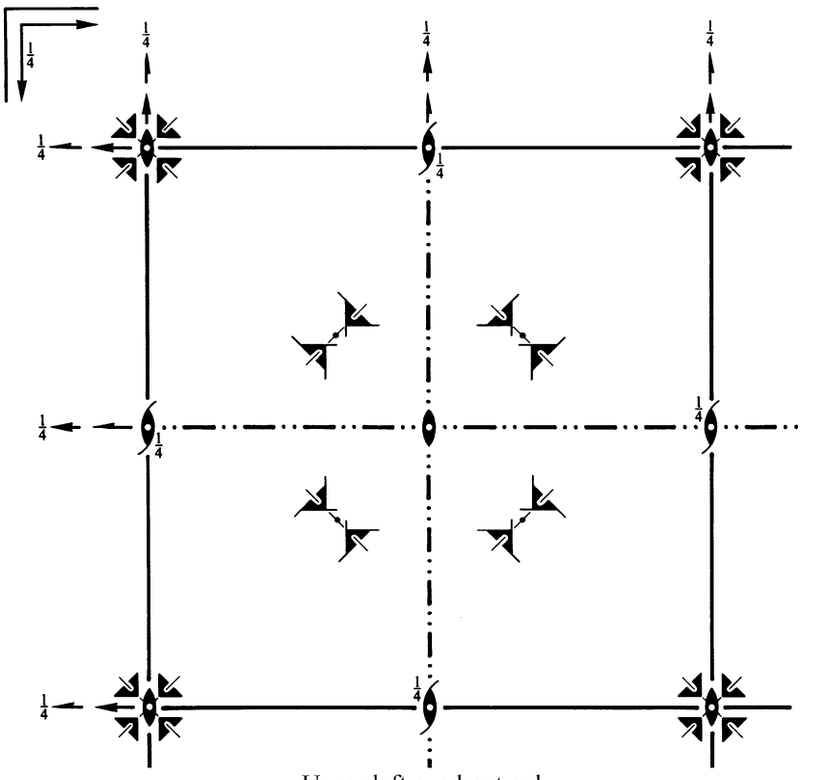
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

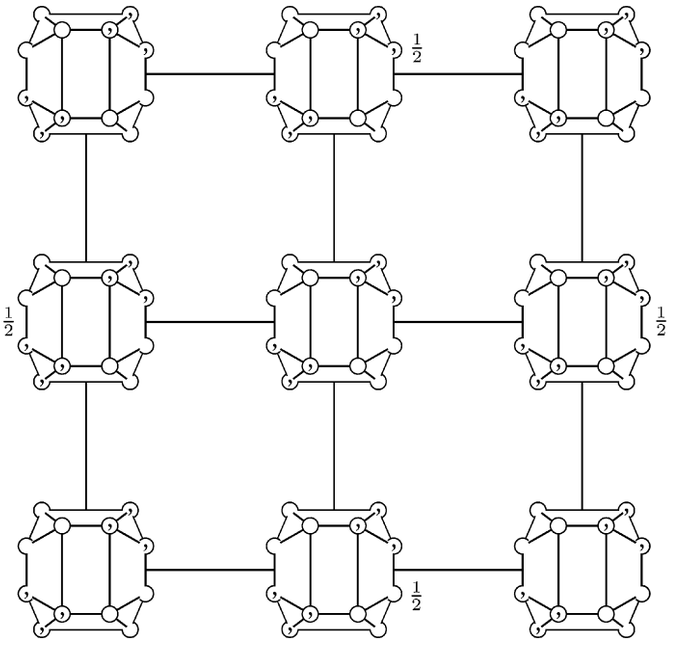
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$Fm\bar{3}$ T_h^3 $m\bar{3}$ Cubic

No. 202 $F2/m\bar{3}$ Patterson symmetry $Fm\bar{3}$



Upper left quadrant only



Origin at centre $(m\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $y \le x$; $z \le \min(\frac{1}{2}-x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $\bar{1}$ $0,0,0$	(14) m $x,y,0$	(15) m $x,0,z$	(16) m $0,y,z$
(17) $\bar{3}^+$ $x,x,x;$ $0,0,0$	(18) $\bar{3}^+$ $\bar{x},x,\bar{x};$ $0,0,0$	(19) $\bar{3}^+$ $x,\bar{x},\bar{x};$ $0,0,0$	(20) $\bar{3}^+$ $\bar{x},\bar{x},x;$ $0,0,0$
(21) $\bar{3}^-$ $x,x,x;$ $0,0,0$	(22) $\bar{3}^-$ $x,\bar{x},\bar{x};$ $0,0,0$	(23) $\bar{3}^-$ $\bar{x},\bar{x},x;$ $0,0,0$	(24) $\bar{3}^-$ $\bar{x},x,\bar{x};$ $0,0,0$

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Symmetry operations *(continued)*

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})\ \ 0,\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)\ \ 0,y,\frac{1}{4}$ (4) $2\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{3},x-\frac{1}{6},x$ (6) $3^+\ \bar{x},x+\frac{1}{2},\bar{x}$ (7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ (8) $3^+\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x+\frac{1}{6},x$ (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) $3^-\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ (12) $3^-\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}\ \ 0,\frac{1}{4},\frac{1}{4}$ (14) $b\ \ x,y,\frac{1}{4}$ (15) $c\ \ x,\frac{1}{4},z$ (16) $n(0,\frac{1}{2},\frac{1}{2})\ \ 0,y,z$
(17) $\bar{3}^+\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$ (18) $\bar{3}^+\ \bar{x}-1,x+\frac{1}{2},\bar{x};\ -\frac{1}{2},0,\frac{1}{2}$ (19) $\bar{3}^+\ x,\bar{x}+\frac{1}{2},\bar{x};\ 0,\frac{1}{2},0$ (20) $\bar{3}^+\ \bar{x}+1,\bar{x}+\frac{1}{2},x;\ \frac{1}{2},0,\frac{1}{2}$
(21) $\bar{3}^-\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$ (22) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$ (23) $\bar{3}^-\ \bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x;\ -\frac{1}{2},\frac{1}{2},0$ (24) $\bar{3}^-\ \bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$ (3) $2\ \ \frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)\ \ x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x-\frac{1}{6},x$ (6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ (7) $3^+\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ (8) $3^+\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x-\frac{1}{6},x-\frac{1}{3},x$ (10) $3^-\ x+\frac{1}{2},\bar{x},\bar{x}$ (11) $3^-\ \bar{x}+\frac{1}{2},\bar{x},x$ (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}\ \ \frac{1}{4},0,\frac{1}{4}$ (14) $a\ \ x,y,\frac{1}{4}$ (15) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,0,z$ (16) $c\ \ \frac{1}{4},y,z$
(17) $\bar{3}^+\ x-\frac{1}{2},x-\frac{1}{2},x;\ 0,0,\frac{1}{2}$ (18) $\bar{3}^+\ \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ 0,0,\frac{1}{2}$ (19) $\bar{3}^+\ x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{2},\frac{1}{2},0$ (20) $\bar{3}^+\ \bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x;\ \frac{1}{2},-\frac{1}{2},0$
(21) $\bar{3}^-\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$ (22) $\bar{3}^-\ x+\frac{1}{2},\bar{x}-1,\bar{x};\ 0,-\frac{1}{2},\frac{1}{2}$ (23) $\bar{3}^-\ \bar{x}+\frac{1}{2},\bar{x}+1,x;\ 0,\frac{1}{2},\frac{1}{2}$ (24) $\bar{3}^-\ \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{1}{2},0,0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2\ \ \frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)\ \ \frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{6},x+\frac{1}{3},x$ (6) $3^+\ \bar{x}+\frac{1}{2},x,\bar{x}$ (7) $3^+\ x+\frac{1}{2},\bar{x},\bar{x}$ (8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ \ x+\frac{1}{3},x+\frac{1}{6},x$ (10) $3^-\ x,\bar{x}+\frac{1}{2},\bar{x}$ (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) $3^-\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}\ \ \frac{1}{4},\frac{1}{4},0$ (14) $n(\frac{1}{2},\frac{1}{2},0)\ \ x,y,0$ (15) $a\ \ x,\frac{1}{4},z$ (16) $b\ \ \frac{1}{4},y,z$
(17) $\bar{3}^+\ x+\frac{1}{2},x,x;\ \frac{1}{2},0,0$ (18) $\bar{3}^+\ \bar{x}-\frac{1}{2},x+1,\bar{x};\ 0,\frac{1}{2},\frac{1}{2}$ (19) $\bar{3}^+\ x-\frac{1}{2},\bar{x}+1,\bar{x};\ 0,\frac{1}{2},-\frac{1}{2}$ (20) $\bar{3}^+\ \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{1}{2},0,0$
(21) $\bar{3}^-\ x,x+\frac{1}{2},x;\ 0,\frac{1}{2},0$ (22) $\bar{3}^-\ x+1,\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{2},0,\frac{1}{2}$ (23) $\bar{3}^-\ \bar{x},\bar{x}+\frac{1}{2},x;\ 0,\frac{1}{2},0$ (24) $\bar{3}^-\ \bar{x}+1,x-\frac{1}{2},\bar{x};\ \frac{1}{2},0,-\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$			Reflection conditions
									h,k,l cyclically permutable
									General:
96	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl: $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl: $h+l=2n$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$			$h00$: $h=2n$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$			
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$			
									Special: as above, plus
48	h	m . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$	no extra conditions
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	
48	g	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	hkl: $h=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x$	
32	f	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x,x,\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
24	e	$m\,m$ 2 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24	d	$2/m$ . .	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h=2n$
8	c	2 3 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl: $h=2n$
4	b	$m\,\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						no extra conditions
4	a	$m\,\bar{3}$.	$0,0,0$						no extra conditions

Symmetry of special projections

Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}\qquad\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

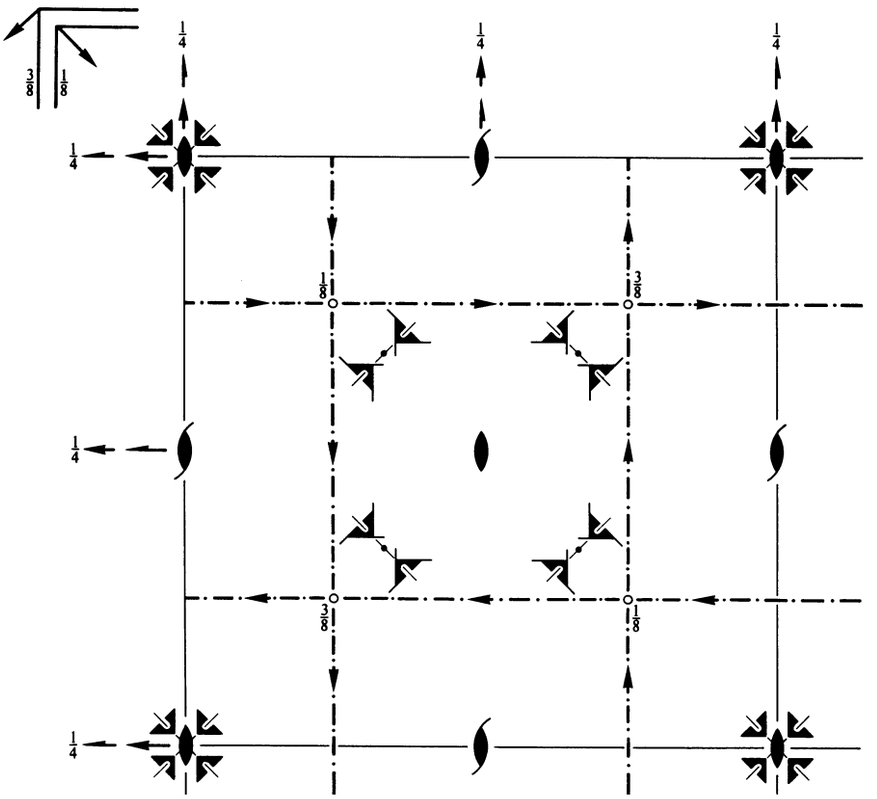
Along [111] $p6$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})\qquad\mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})\qquad\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

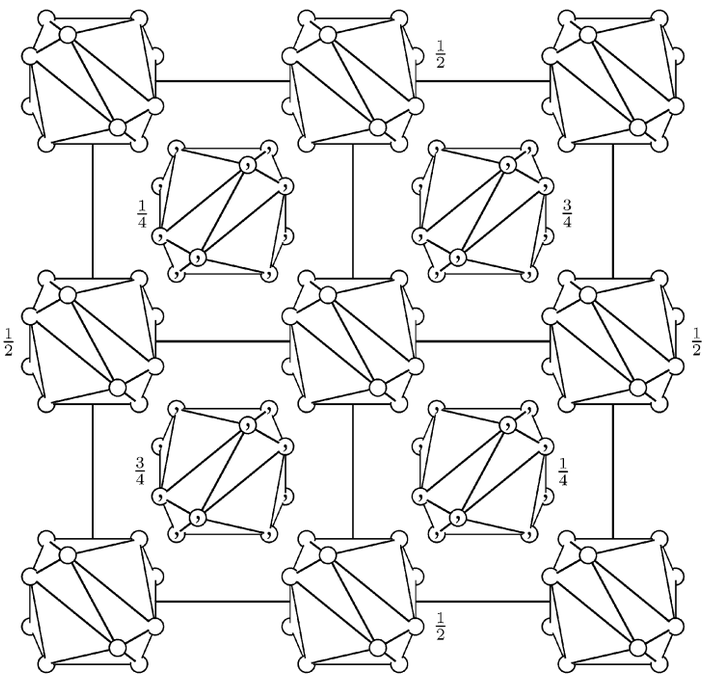
$F\,d\,\bar{3}$ T_h^4 $m\bar{3}$ Cubic

No. 203 $F\,2/d\,\bar{3}$ Patterson symmetry $F\,m\,\bar{3}$

ORIGIN CHOICE 1



Upper left quadrant only



Origin at 23, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre $(\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2}-x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $\bar{1}$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$	(14) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,\frac{1}{8}$	(15) $d(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},z$	(16) $d(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,z$
(17) $\bar{3}^+$ x,x,x; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$	(18) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$; $-\frac{1}{8},\frac{1}{8},\frac{3}{8}$	(19) $\bar{3}^+$ $x,\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{8},\frac{3}{8},-\frac{1}{8}$	(20) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x},x$; $\frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(21) $\bar{3}^-$ x,x,x; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$	(22) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; $\frac{1}{8},-\frac{1}{8},\frac{3}{8}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; $-\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(24) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ 0,$\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ 0,$y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$	(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}$ $\frac{1}{8},\frac{3}{8},\frac{3}{8}$	(14) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{3}{8}$	(15) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{3}{8},z$	(16) $d(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,z$
(17) $\bar{3}^+$ $x,x+\frac{1}{2},x$; $\frac{1}{8},\frac{5}{8},\frac{1}{8}$	(18) $\bar{3}^+$ $\bar{x}-\frac{3}{2},x+1,\bar{x}$; $-\frac{5}{8},\frac{1}{8},\frac{7}{8}$	(19) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}$; $\frac{1}{8},\frac{7}{8},-\frac{1}{8}$	(20) $\bar{3}^+$ $\bar{x}+\frac{3}{2},\bar{x}+\frac{1}{2},x$; $\frac{7}{8},-\frac{1}{8},\frac{5}{8}$
(21) $\bar{3}^-$ $x-\frac{1}{2},x-\frac{1}{2},x$; $\frac{1}{8},\frac{1}{8},\frac{5}{8}$	(22) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}$; $\frac{1}{8},-\frac{1}{8},\frac{7}{8}$	(23) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+1,x$; $-\frac{5}{8},\frac{7}{8},\frac{1}{8}$	(24) $\bar{3}^-$ $\bar{x}+1,x+\frac{1}{2},\bar{x}$; $\frac{7}{8},\frac{5}{8},-\frac{1}{8}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}$,0,z	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ x,0,$\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$	(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}$ $\frac{3}{8},\frac{1}{8},\frac{3}{8}$	(14) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{3}{8}$	(15) $d(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},z$	(16) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{3}{8},y,z$
(17) $\bar{3}^+$ $x-\frac{1}{2},x-\frac{1}{2},x$; $\frac{1}{8},\frac{1}{8},\frac{5}{8}$	(18) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{1}{8},\frac{1}{8},\frac{7}{8}$	(19) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+1,\bar{x}$; $\frac{5}{8},\frac{7}{8},-\frac{1}{8}$	(20) $\bar{3}^+$ $\bar{x}+1,\bar{x}-\frac{1}{2},x$; $\frac{7}{8},-\frac{5}{8},\frac{1}{8}$
(21) $\bar{3}^-$ $x+\frac{1}{2},x,x$; $\frac{5}{8},\frac{1}{8},\frac{1}{8}$	(22) $\bar{3}^-$ $x+1,\bar{x}-\frac{3}{2},\bar{x}$; $\frac{1}{8},-\frac{5}{8},\frac{7}{8}$	(23) $\bar{3}^-$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{3}{2},x$; $-\frac{1}{8},\frac{7}{8},\frac{5}{8}$	(24) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{7}{8},\frac{1}{8},-\frac{1}{8}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$	(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $\bar{1}$ $\frac{3}{8},\frac{3}{8},\frac{1}{8}$	(14) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,\frac{1}{8}$	(15) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{3}{8},z$	(16) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{3}{8},y,z$
(17) $\bar{3}^+$ $x+\frac{1}{2},x,x$; $\frac{5}{8},\frac{1}{8},\frac{1}{8}$	(18) $\bar{3}^+$ $\bar{x}-1,x+\frac{3}{2},\bar{x}$; $-\frac{1}{8},\frac{5}{8},\frac{7}{8}$	(19) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+\frac{3}{2},\bar{x}$; $\frac{1}{8},\frac{7}{8},-\frac{5}{8}$	(20) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{7}{8},-\frac{1}{8},\frac{1}{8}$
(21) $\bar{3}^-$ $x,x+\frac{1}{2},x$; $\frac{1}{8},\frac{5}{8},\frac{1}{8}$	(22) $\bar{3}^-$ $x+\frac{3}{2},\bar{x}-1,\bar{x}$; $\frac{5}{8},-\frac{1}{8},\frac{7}{8}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{1}{8},\frac{7}{8},\frac{1}{8}$	(24) $\bar{3}^-$ $\bar{x}+\frac{3}{2},x-\frac{1}{2},\bar{x}$; $\frac{7}{8},\frac{1}{8},-\frac{5}{8}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
96	g	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$ (9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$ (13) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$ (14) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$ (15) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{1}{4}$ (16) $\bar{x}+\frac{1}{4},y+\frac{1}{4},z+\frac{1}{4}$ (17) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$ (18) $\bar{z}+\frac{1}{4},x+\frac{1}{4},y+\frac{1}{4}$ (19) $z+\frac{1}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$ (20) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{1}{4}$ (21) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$ (22) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{1}{4}$ (23) $\bar{y}+\frac{1}{4},z+\frac{1}{4},x+\frac{1}{4}$ (24) $y+\frac{1}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$	h,k,l cyclically permutable General: hkl: $h+k=2n$ and $h+l,k+l=2n$ $0kl$: $k+l=4n$ and $k,l=2n$ hhl: $h+l=2n$ $h00$: $h=4n$
				Special: as above, plus
48	f	2 . .	$x,0,0$ $\bar{x}+\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\bar{x},0,0$ $x+\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $0,x,0$ $\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$ $0,\bar{x},0$ $\frac{1}{4},x+\frac{1}{4},\frac{1}{4}$ $0,0,x$ $\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{4}$ $0,0,\bar{x}$ $\frac{1}{4},\frac{1}{4},x+\frac{1}{4}$	hkl: $h=2n+1$ or $h+k+l=4n$
32	e	. 3 .	x,x,x $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$ $\bar{x},\bar{x},x$ $x+\frac{1}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$ $\bar{x},x,\bar{x}$ $x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{1}{4}$ $x,\bar{x},\bar{x}$ $\bar{x}+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$	no extra conditions
16	d	. $\bar{3}$.	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$ $\frac{3}{8},\frac{3}{8},\frac{5}{8}$ $\frac{3}{8},\frac{5}{8},\frac{3}{8}$ $\frac{5}{8},\frac{3}{8},\frac{3}{8}$	hkl: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	. $\bar{3}$.	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{7}{8},\frac{7}{8},\frac{1}{8}$ $\frac{7}{8},\frac{1}{8},\frac{7}{8}$ $\frac{1}{8},\frac{7}{8},\frac{7}{8}$	
8	b	2 3 .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$	hkl: $h=2n+1$ or $h+k+l=4n$
8	a	2 3 .	0,0,0 $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	

Symmetry of special projections

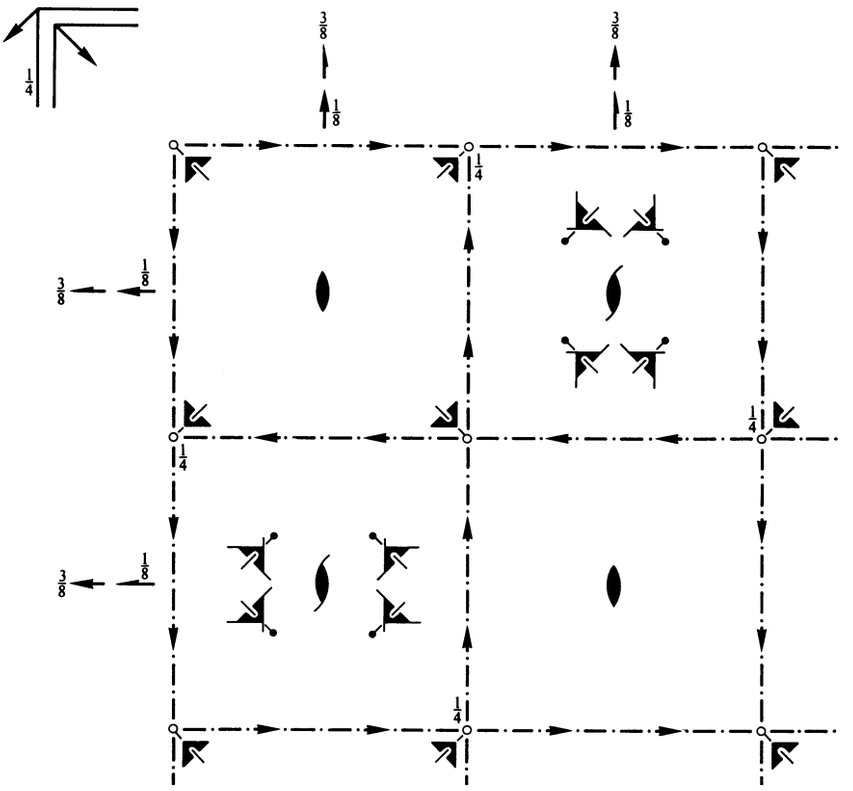
Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

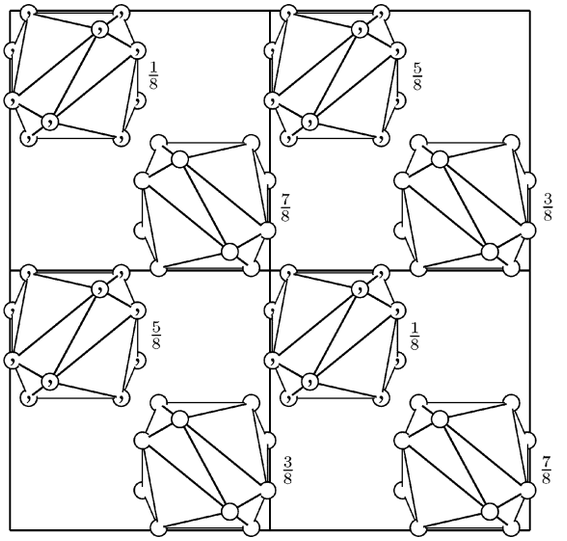
Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{8}$

No. 203 $F\,2/d\,\bar{3}$ Patterson symmetry $F\,m\,\bar{3}$

ORIGIN CHOICE 2



Upper left quadrant only



Origin at centre $(\bar{3})$, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from 23

Asymmetric unit $-\frac{1}{8} \le x \le \frac{3}{8}$; $-\frac{1}{8} \le y \le \frac{1}{8}$; $-\frac{3}{8} \le z \le \frac{1}{8}$; $y \le \min(x, \frac{1}{4}-x)$; $-y-\frac{1}{4} \le z \le y$

Vertices $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{3}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},-\frac{3}{8}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 $\frac{3}{8},\frac{3}{8},z$	(3) 2 $\frac{3}{8},y,\frac{3}{8}$	(4) 2 $x,\frac{3}{8},\frac{3}{8}$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x+\frac{3}{4},\bar{x}$	(7) 3^+ $x+\frac{3}{4},\bar{x},\bar{x}$	(8) 3^+ $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$
(9) 3^- x,x,x	(10) 3^- $x+\frac{3}{4},\bar{x},\bar{x}$	(11) 3^- $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$	(12) 3^- $\bar{x},x+\frac{3}{4},\bar{x}$
(13) $\bar{1}$ 0,0,0	(14) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,0$	(15) $d(\frac{1}{4},0,\frac{1}{4})$ $x,0,z$	(16) $d(0,\frac{1}{4},\frac{1}{4})$ $0,y,z$
(17) $\bar{3}^+$ x,x,x; 0,0,0	(18) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{4},\bar{x}$; $-\frac{1}{4},0,\frac{1}{4}$	(19) $\bar{3}^+$ $x-\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$; $0,\frac{1}{4},-\frac{1}{4}$	(20) $\bar{3}^+$ $\bar{x}+\frac{1}{4},\bar{x}-\frac{1}{4},x$; $\frac{1}{4},-\frac{1}{4},0$
(21) $\bar{3}^-$ x,x,x; 0,0,0	(22) $\bar{3}^-$ $x+\frac{1}{4},\bar{x}-\frac{1}{2},\bar{x}$; $0,-\frac{1}{4},\frac{1}{4}$	(23) $\bar{3}^-$ $\bar{x}-\frac{1}{4},\bar{x}+\frac{1}{4},x$; $-\frac{1}{4},\frac{1}{4},0$	(24) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x-\frac{1}{4},\bar{x}$; $\frac{1}{4},0,-\frac{1}{4}$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{3}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{3}{8},y,\frac{1}{8}$	(4) 2 $x,\frac{1}{8},\frac{1}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$	(6) 3^+ $\bar{x},x+\frac{1}{4},\bar{x}$	(7) 3^+ $x+\frac{3}{4},\bar{x}-\frac{1}{2},\bar{x}$	(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{5}{12},\bar{x}+\frac{7}{12},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$	(10) 3^- $x+\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{7}{12},\bar{x}$
(13) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$	(14) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{1}{4}$	(15) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{1}{4},z$	(16) $d(0,\frac{3}{4},\frac{3}{4})$ $0,y,z$
(17) $\bar{3}^+$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$	(18) $\bar{3}^+$ $\bar{x}-\frac{3}{2},x+\frac{3}{4},\bar{x}$; $-\frac{3}{4},0,\frac{3}{4}$	(19) $\bar{3}^+$ $x-\frac{1}{4},\bar{x}+1,\bar{x}$; $0,\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+$ $\bar{x}+\frac{5}{4},\bar{x}+\frac{1}{4},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{2}$
(21) $\bar{3}^-$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$	(22) $\bar{3}^-$ $x+\frac{3}{4},\bar{x}-1,\bar{x}$; $0,-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^-$ $\bar{x}-\frac{3}{4},\bar{x}+\frac{3}{4},x$; $-\frac{3}{4},\frac{3}{4},0$	(24) $\bar{3}^-$ $\bar{x}+1,x+\frac{1}{4},\bar{x}$; $\frac{3}{4},\frac{1}{2},-\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{8},\frac{3}{8},z$	(3) 2 $\frac{1}{8},y,\frac{1}{8}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{3}{8},\frac{1}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$	(6) 3^+ $\bar{x}+\frac{1}{2},x+\frac{1}{4},\bar{x}$	(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{7}{12},\bar{x}-\frac{1}{6},\bar{x}$	(8) 3^+ $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$	(10) 3^- $x+\frac{1}{4},\bar{x},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{7}{12},\bar{x}+\frac{5}{12},x$	(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{3}{4},\bar{x}$
(13) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$	(14) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{1}{4}$	(15) $d(\frac{3}{4},0,\frac{3}{4})$ $x,0,z$	(16) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{1}{4},y,z$
(17) $\bar{3}^+$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$	(18) $\bar{3}^+$ $\bar{x}-1,x+\frac{3}{4},\bar{x}$; $-\frac{1}{4},0,\frac{3}{4}$	(19) $\bar{3}^+$ $x+\frac{1}{4},\bar{x}+1,\bar{x}$; $\frac{1}{2},\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+$ $\bar{x}+\frac{3}{4},\bar{x}-\frac{3}{4},x$; $\frac{3}{4},-\frac{3}{4},0$
(21) $\bar{3}^-$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$	(22) $\bar{3}^-$ $x+\frac{3}{4},\bar{x}-\frac{3}{2},\bar{x}$; $0,-\frac{3}{4},\frac{3}{4}$	(23) $\bar{3}^-$ $\bar{x}+\frac{1}{4},\bar{x}+\frac{5}{4},x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{2}$	(24) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{4},\bar{x}$; $\frac{3}{4},0,-\frac{1}{4}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{8},\frac{1}{8},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{8},y,\frac{3}{8}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{8},\frac{3}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$	(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{5}{12},\bar{x}$	(7) 3^+ $x+\frac{1}{4},\bar{x},\bar{x}$	(8) 3^+ $\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{5}{12},\bar{x}+\frac{1}{6},\bar{x}$	(11) 3^- $\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x$	(12) 3^- $\bar{x},x+\frac{1}{4},\bar{x}$
(13) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(14) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,0$	(15) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{1}{4},z$	(16) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{1}{4},y,z$
(17) $\bar{3}^+$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$	(18) $\bar{3}^+$ $\bar{x}-1,x+\frac{5}{4},\bar{x}$; $-\frac{1}{4},\frac{1}{2},\frac{3}{4}$	(19) $\bar{3}^+$ $x-\frac{3}{4},\bar{x}+\frac{3}{2},\bar{x}$; $0,\frac{3}{4},-\frac{3}{4}$	(20) $\bar{3}^+$ $\bar{x}+\frac{3}{4},\bar{x}-\frac{1}{4},x$; $\frac{3}{4},-\frac{1}{4},0$
(21) $\bar{3}^-$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$	(22) $\bar{3}^-$ $x+\frac{5}{4},\bar{x}-1,\bar{x}$; $\frac{1}{2},-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^-$ $\bar{x}-\frac{1}{4},\bar{x}+\frac{3}{4},x$; $-\frac{1}{4},\frac{3}{4},0$	(24) $\bar{3}^-$ $\bar{x}+\frac{3}{2},x-\frac{3}{4},\bar{x}$; $\frac{3}{4},0,-\frac{3}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+	(0,½,½)+	(½,0,½)+	(½,½,0)+	Reflection conditions
							h,k,l cyclically permutable
							General:
96	g	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},z$	(3) $\bar{x}+\frac{3}{4},y,\bar{z}+\frac{3}{4}$	(4) $x,\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4},y$	(8) $\bar{z}+\frac{3}{4},x,\bar{y}+\frac{3}{4}$	$0kl$: $k+l=4n$, $k,l=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{3}{4},z,\bar{x}+\frac{3}{4}$	(11) $y,\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4},x$	hhl: $h+l=2n$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{4},y+\frac{1}{4},\bar{z}$	(15) $x+\frac{1}{4},\bar{y},z+\frac{1}{4}$	(16) $\bar{x},y+\frac{1}{4},z+\frac{1}{4}$	$h00$: $h=4n$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x+\frac{1}{4},y+\frac{1}{4}$	(19) $z+\frac{1}{4},x+\frac{1}{4},\bar{y}$	(20) $z+\frac{1}{4},\bar{x},y+\frac{1}{4}$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y+\frac{1}{4},\bar{z},x+\frac{1}{4}$	(23) $\bar{y},z+\frac{1}{4},x+\frac{1}{4}$	(24) $y+\frac{1}{4},z+\frac{1}{4},\bar{x}$	
							Special: as above, plus
48	f	2 . .	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{5}{8},\frac{1}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{1}{8},\bar{x}+\frac{3}{4},\frac{5}{8}$	$\frac{1}{8},\frac{1}{8},x$	$\frac{5}{8},\frac{1}{8},\bar{x}+\frac{3}{4}$	hkl: $h=2n+1$
			$\bar{x},\frac{7}{8},\frac{7}{8}$	$x+\frac{1}{4},\frac{3}{8},\frac{7}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$\frac{7}{8},x+\frac{1}{4},\frac{3}{8}$	$\frac{7}{8},\frac{7}{8},\bar{x}$	$\frac{3}{8},\frac{7}{8},x+\frac{1}{4}$	or $h+k+l=4n$
32	e	. 3 .	x,x,x	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$	$\bar{x}+\frac{3}{4},x,\bar{x}+\frac{3}{4}$	$x,\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{4},x+\frac{1}{4},\bar{x}$	$x+\frac{1}{4},\bar{x},x+\frac{1}{4}$	$\bar{x},x+\frac{1}{4},x+\frac{1}{4}$			
16	d	. $\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{1}{4}$			hkl: $h=2n+1$
16	c	. $\bar{3}$.	$0,0,0$	$\frac{3}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{3}{4}$	$0,\frac{3}{4},\frac{3}{4}$			or $h,k,l=4n+2$
									or $h,k,l=4n$
8	b	2 3 .	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$					hkl: $h=2n+1$
8	a	2 3 .	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$					or $h+k+l=4n$

Symmetry of special projections

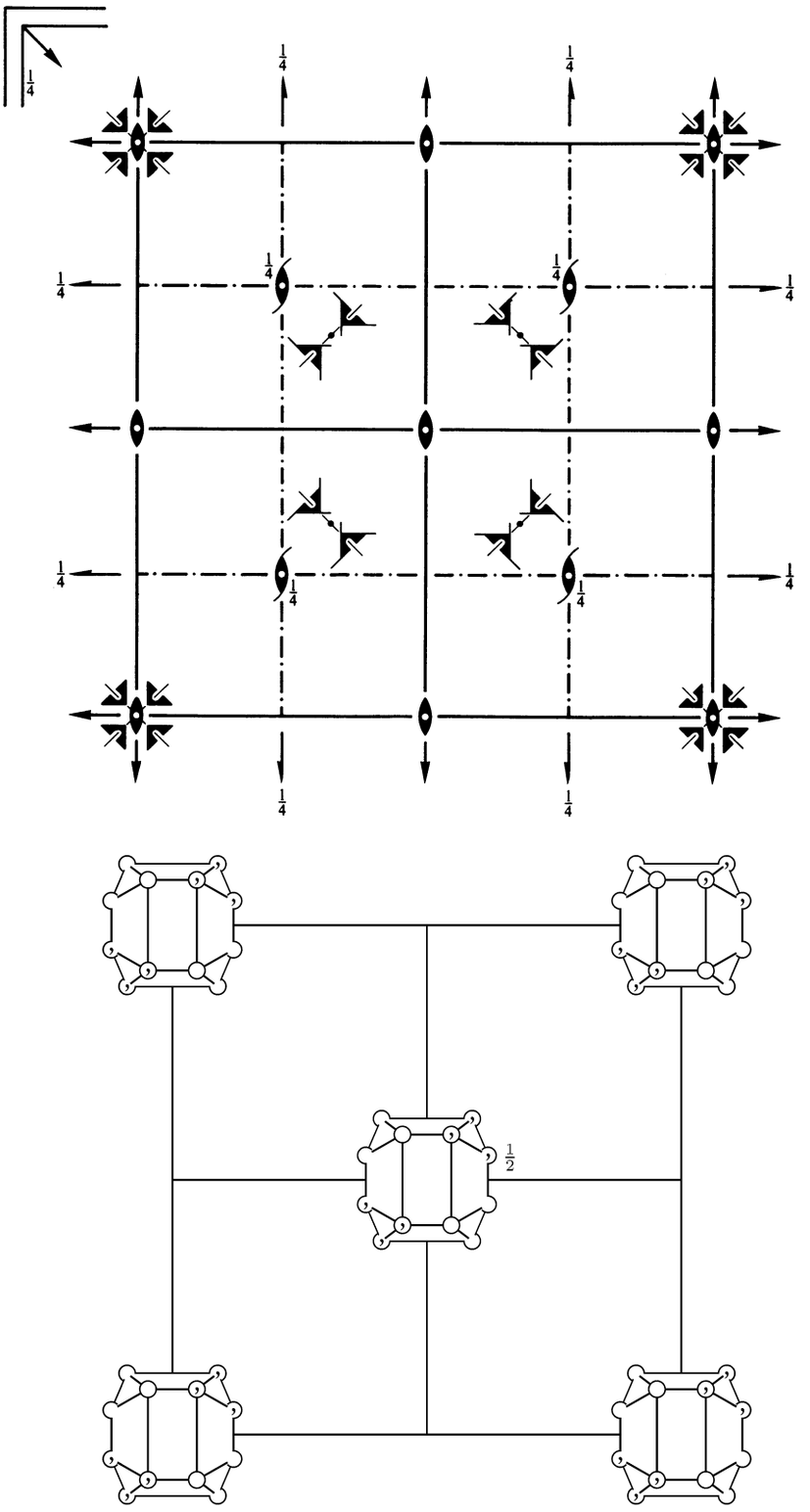
Along [001] $c2mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{8},\frac{1}{8},z$

Along [111] $p6$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$Im\bar{3}$ T_h^5 $m\bar{3}$ Cubic

No. 204 $I2/m\bar{3}$ Patterson symmetry $Im\bar{3}$



Origin at centre $(m\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $\bar{1}$ 0,0,0	(14) m x,y,0	(15) m x,0,z	(16) m 0,y,z
(17) $\bar{3}^+$ x,x,x; 0,0,0	(18) $\bar{3}^+$ $\bar{x},x,\bar{x}$; 0,0,0	(19) $\bar{3}^+$ $x,\bar{x},\bar{x}$; 0,0,0	(20) $\bar{3}^+$ $\bar{x},\bar{x},x$; 0,0,0
(21) $\bar{3}^-$ x,x,x; 0,0,0	(22) $\bar{3}^-$ $x,\bar{x},\bar{x}$; 0,0,0	(23) $\bar{3}^-$ $\bar{x},\bar{x},x$; 0,0,0	(24) $\bar{3}^-$ $\bar{x},x,\bar{x}$; 0,0,0

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(14) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(15) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(16) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(17) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(18) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(19) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}$; $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(20) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(21) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(22) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(24) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	Coordinates $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
								h,k,l cyclically permutable
								General:
48	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$		hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $h00$: $h=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$		
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$		
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x,y,\bar{z}$	(15) $x,\bar{y},z$	(16) $\bar{x},y,z$		
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z},x,y$	(19) $z,x,\bar{y}$	(20) $z,\bar{x},y$		
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z},x$	(23) $\bar{y},z,x$	(24) $y,z,\bar{x}$		
								Special: as above, plus
24	g	m . .	$0,y,z$ $\bar{z},0,y$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$	$0,y,\bar{z}$ $y,z,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$	$z,0,y$ $y,\bar{z},0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$	no extra conditions
16	f	. 3 .	x,x,x $\bar{x},\bar{x},\bar{x}$	$\bar{x},\bar{x},x$ $x,x,\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$			no extra conditions
12	e	$m\,m\,2$ . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	no extra conditions
12	d	$m\,m\,2$ . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
8	c	. $\bar{3}$.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $k,l=2n$
6	b	$m\,m\,m$ . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	a	$m\,\bar{3}$.	$0,0,0$						no extra conditions

Symmetry of special projections

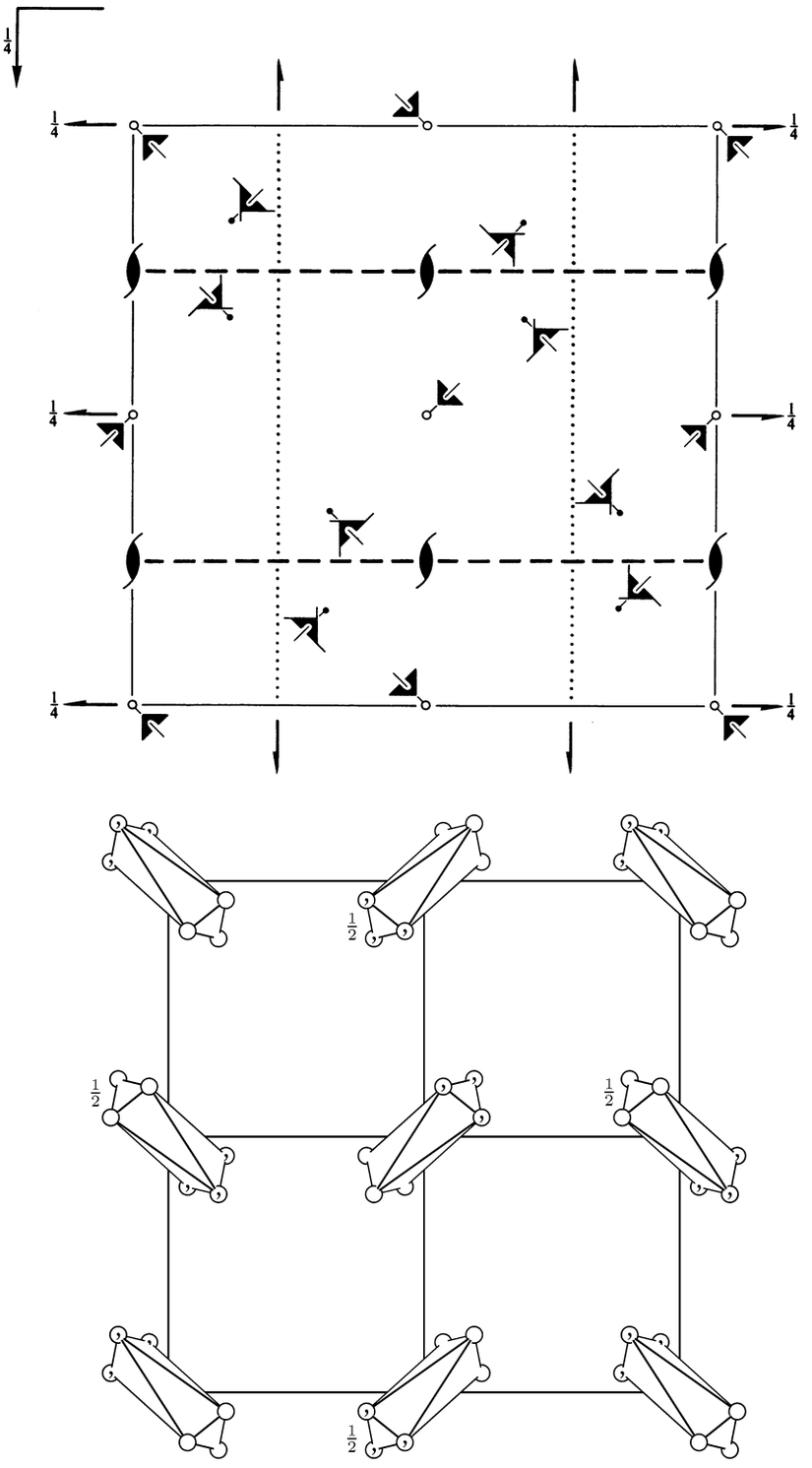
Along [001] $c2mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$Pa\bar{3}$ T_h^6 $m\bar{3}$ Cubic

No. 205 $P2_1/a\bar{3}$ Patterson symmetry $Pm\bar{3}$



Origin at centre $(\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x,y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}$ 0,0,0	(14) a $x,y,\frac{1}{4}$	(15) c $x,\frac{1}{4},z$	(16) b $\frac{1}{4},y,z$
(17) $\bar{3}^+$ $x,x,x;$ 0,0,0	(18) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x};$ $0,\frac{1}{2},\frac{1}{2}$	(19) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};$ $\frac{1}{2},\frac{1}{2},0$	(20) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x;$ $\frac{1}{2},0,\frac{1}{2}$
(21) $\bar{3}^-$ $x,x,x;$ 0,0,0	(22) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};$ $0,0,\frac{1}{2}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x;$ $0,\frac{1}{2},0$	(24) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x};$ $\frac{1}{2},0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l cyclically permutable
							General:
24	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(15) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(19) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(20) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(24) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	
							Special: as above, plus
8	c	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x$	
4	b	. $\bar{3}$.	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
4	a	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+k,h+l,k+l=2n$

Symmetry of special projections

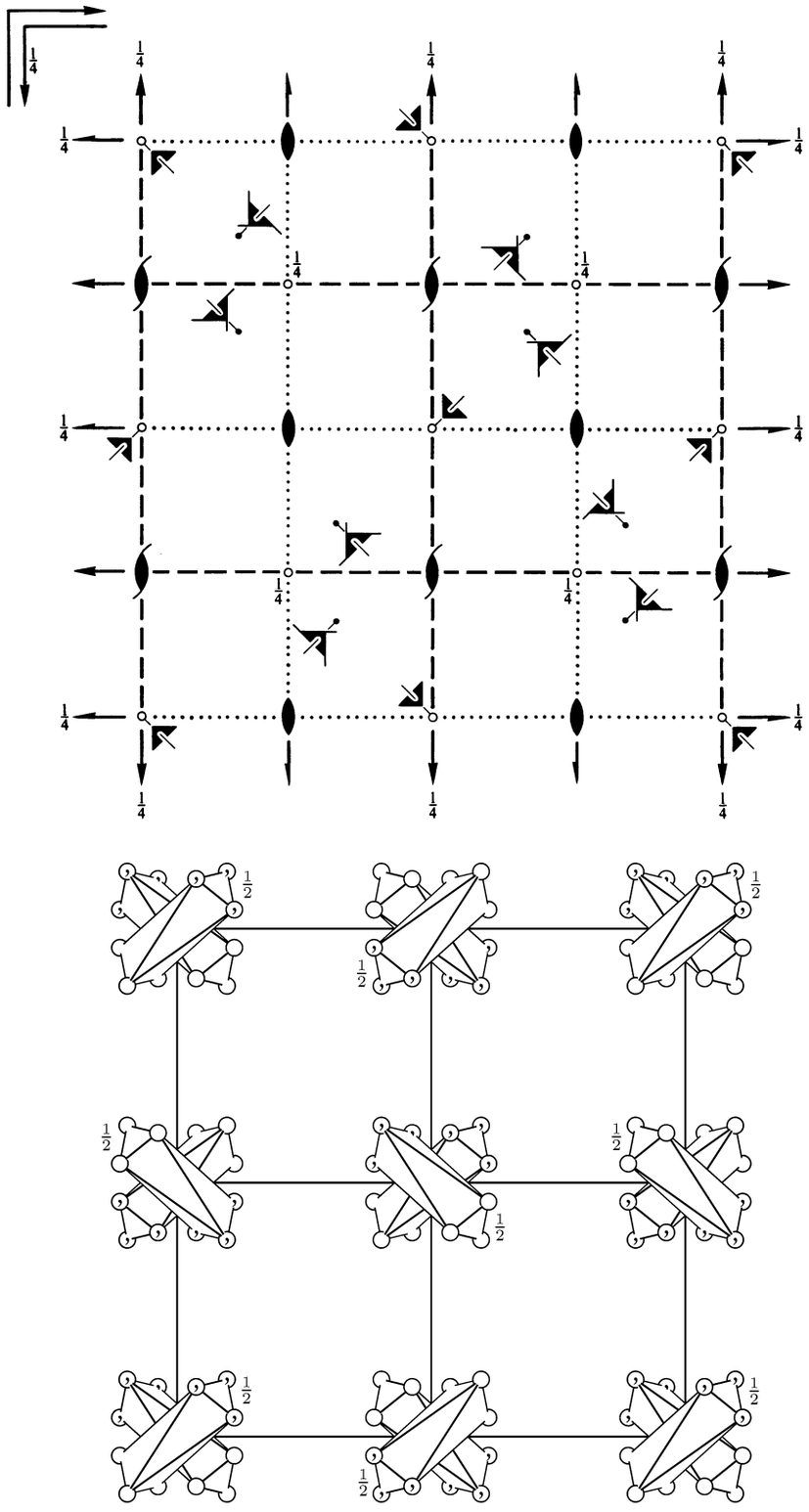
Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2gg$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$Ia\bar{3}$ T_h^7 $m\bar{3}$ Cubic

No. 206 $I2_1/a\bar{3}$ Patterson symmetry $Im\bar{3}$



Origin at centre $(\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}; \quad z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad 0,\frac{1}{2},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}$ 0,0,0	(14) a $x,y,\frac{1}{4}$	(15) c $x,\frac{1}{4},z$	(16) b $\frac{1}{4},y,z$
(17) $\bar{3}^+$ $x,x,x;$ 0,0,0	(18) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x};$ $0,\frac{1}{2},\frac{1}{2}$	(19) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};$ $\frac{1}{2},\frac{1}{2},0$	(20) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x;$ $\frac{1}{2},0,\frac{1}{2}$
(21) $\bar{3}^-$ $x,x,x;$ 0,0,0	(22) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};$ $0,0,\frac{1}{2}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x;$ $0,\frac{1}{2},0$	(24) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x};$ $\frac{1}{2},0,0$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) 2 $0,\frac{1}{4},z$	(3) 2 $\frac{1}{4},y,0$	(4) 2 $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(14) b $x,y,0$	(15) a $x,0,z$	(16) c $0,y,z$
(17) $\bar{3}^+$ $x,x,x;$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(18) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x,\bar{x};$ $-\frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(19) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x};$ $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$	(20) $\bar{3}^+$ $\bar{x},\bar{x}-\frac{1}{2},x;$ $\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$
(21) $\bar{3}^-$ $x,x,x;$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(22) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};$ $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$	(23) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x;$ $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(24) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x};$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
							h,k,l cyclically permutable
							General:
48	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	hhl: $l=2n$
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(15) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	$h00$: $h=2n$
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(19) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(20) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(24) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	
							Special: as above, plus
24	d	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$	no extra conditions
			$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$\frac{3}{4},\bar{x},0$	$\frac{1}{4},x+\frac{1}{2},0$	$0,\frac{3}{4},\bar{x}$	$0,\frac{1}{4},x+\frac{1}{2}$	
16	c	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$			no extra conditions
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x$			
8	b	. $\bar{3}$.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			hkl: $k,l=2n$
8	a	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl: $k,l=2n$

Symmetry of special projections

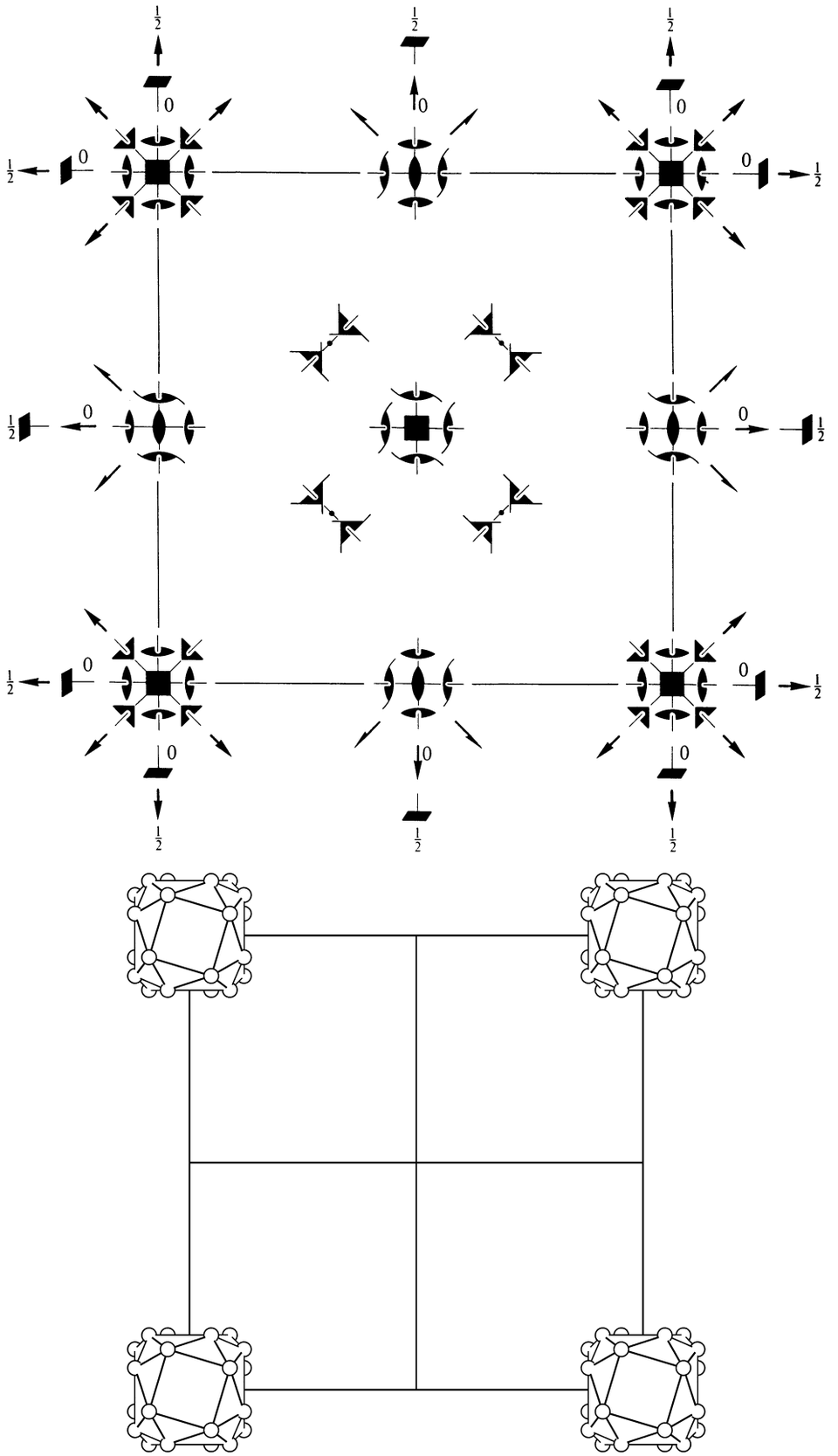
Along [001] $p2mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mg$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P432$ O^1 432 Cubic

No. 207 $P432$ Patterson symmetry $Pm\bar{3}m$



Origin at 432

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad y \le \min(x, 1-x); \quad z \le y$

Vertices $0,0,0 \quad 1,0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$	(14) 2 $x,\bar{x},0$	(15) 4^- $0,0,z$	(16) 4^+ $0,0,z$
(17) 4^- $x,0,0$	(18) 2 $0,y,y$	(19) 2 $0,y,\bar{y}$	(20) 4^+ $x,0,0$
(21) 4^+ $0,y,0$	(22) 2 $x,0,x$	(23) 4^- $0,y,0$	(24) 2 $\bar{x},0,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l permutable
									General:
24	k	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$			
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$			
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$			
									Special: no extra conditions
12	j	. . 2	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$	
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$	
12	i	. . 2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
12	h	2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
			$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$	$0,\frac{1}{2},x$	
8	g	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
6	f	4 . .	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	
6	e	4 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
3	d	4 2 .2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$				
3	c	4 2 .2	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				
1	b	4 3 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
1	a	4 3 2	$0,0,0$						

Symmetry of special projections

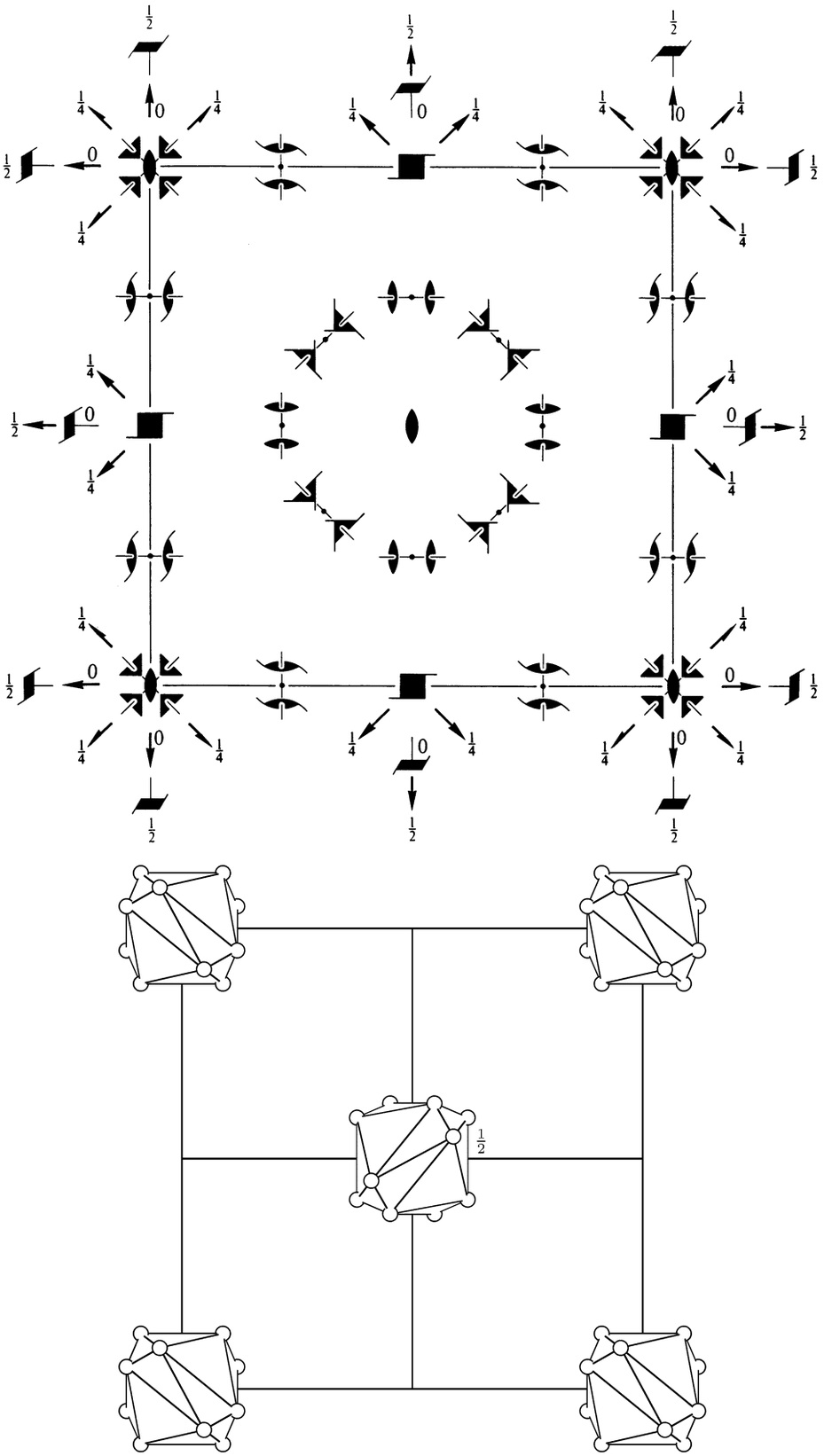
Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [111] $p3m1$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$P4_232$ O^2 432 Cubic

No. 208 $P4_232$ Patterson symmetry $Pm\bar{3}m$



Origin at 2 3

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $\max(-x, x-\frac{1}{2}, -y, y-\frac{1}{2}) \le z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

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Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$	(16) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,y$	(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0)$ $x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0)$ $0,y,\frac{1}{2}$	(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
									h,k,l permutable
									General:
24	m	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			$h00$: $h=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$			
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$			
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$			
									Special: as above, plus
12	l	. . 2	$\frac{1}{4},y,y+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},y$ $y,y+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{y},y+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},y,\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{3}{4},y$ $y,\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$			no extra conditions
12	k	. . 2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},y,y+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},y$ $y,y+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$			no extra conditions
12	j	2 . .	$x,\frac{1}{2},0$ $0,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$ $0,\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,x$ $\frac{1}{2},0,\bar{x}+\frac{1}{2}$	$\frac{1}{2},0,\bar{x}$ $\frac{1}{2},0,x+\frac{1}{2}$	hkl: $h=2n$ hhl: $l=2n$
12	i	2 . .	$x,0,\frac{1}{2}$ $\frac{1}{2},x+\frac{1}{2},0$	$\bar{x},0,\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x,0$ $x+\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\bar{x},0$ $\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},x$ $0,\frac{1}{2},\bar{x}+\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$ $0,\frac{1}{2},x+\frac{1}{2}$	hkl: $h=2n$ hhl: $l=2n$
12	h	2 . .	$x,0,0$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,0$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\bar{x},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,x$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$0,0,\bar{x}$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	hkl: $h+k+l=2n$
8	g	. 3 .	x,x,x $\bar{x},x,\bar{x}$ $x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{x},x$ $x,\bar{x},\bar{x}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					$0kl$: $k+l=2n$
6	f	2 . 2 2	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k+l=2n$ or $h=2n+1,k=4n$ and $l=4n+2$
6	e	2 . 2 2	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	
6	d	2 2 2 . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl: $h+k+l=2n$
4	c	. 3 2	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$			hkl: $h+k,h+l,k+l=2n$
4	b	. 3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $h+k,h+l,k+l=2n$
2	a	2 3 .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl: $h+k+l=2n$

Symmetry of special projections

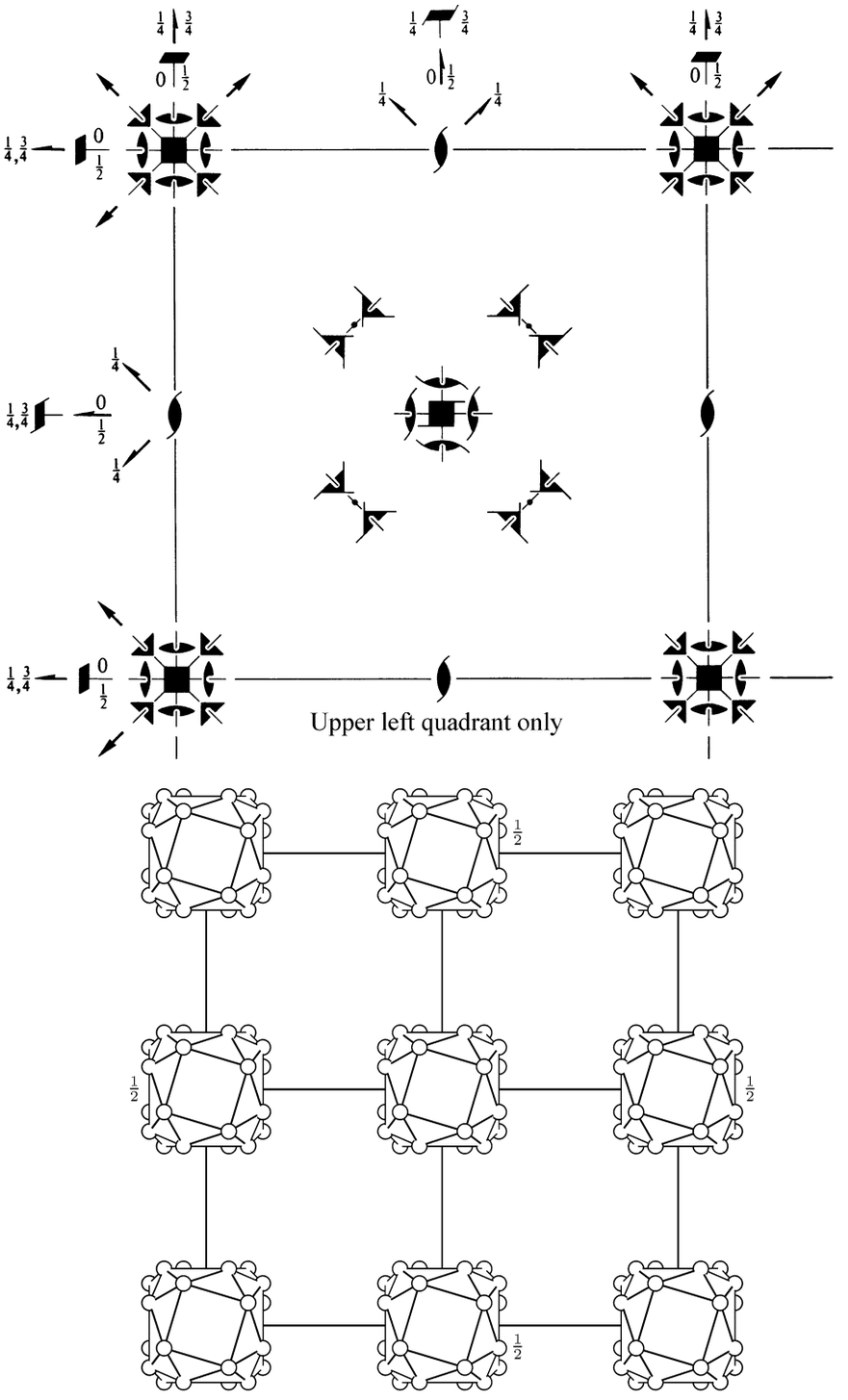
Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,\frac{1}{2},z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{4}$

$F432$ O^3 432 Cubic

No. 209 $F432$ Patterson symmetry $Fm\bar{3}m$



Origin at 432

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2}-x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$	(14) 2 $x,\bar{x},0$	(15) 4^- $0,0,z$	(16) 4^+ $0,0,z$
(17) 4^- $x,0,0$	(18) 2 $0,y,y$	(19) 2 $0,y,\bar{y}$	(20) 4^+ $x,0,0$
(21) 4^+ $0,y,0$	(22) 2 $x,0,x$	(23) 4^- $0,y,0$	(24) 2 $\bar{x},0,x$

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Symmetry operations *(continued)*

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$ (6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$ (7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$ (8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$ (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ (12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x+\frac{1}{4},\frac{1}{4}$ (14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$ (15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$ (16) $4^+(0,0,\frac{1}{2})$ $-\frac{1}{4},\frac{1}{4},z$
(17) 4^- $x,\frac{1}{2},0$ (18) $2(0,\frac{1}{2},\frac{1}{2})$ $0,y,y$ (19) 2 $0,y+\frac{1}{2},\bar{y}$ (20) 4^+ $x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (22) $2(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},\frac{1}{4},x$ (23) $4^-(0,\frac{1}{2},0)$ $-\frac{1}{4},y,\frac{1}{4}$ (24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},\frac{1}{4},x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) 2 $\frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$ (6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$ (7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ (8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$ (10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$ (11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$ (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x-\frac{1}{4},\frac{1}{4}$ (14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$ (15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},-\frac{1}{4},z$ (16) $4^+(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$ (18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y-\frac{1}{4},y$ (19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$ (20) $4^+(\frac{1}{2},0,0)$ $x,-\frac{1}{4},\frac{1}{4}$
(21) 4^+ $\frac{1}{2},y,0$ (22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,0,x$ (23) 4^- $0,y,\frac{1}{2}$ (24) 2 $\bar{x}+\frac{1}{2},0,x$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$ (6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$ (7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$ (8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$ (10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$ (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$ (14) 2 $x,\bar{x}+\frac{1}{2},0$ (15) 4^- $\frac{1}{2},0,z$ (16) 4^+ $0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{4},-\frac{1}{4}$ (18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},y$ (19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$ (20) $4^+(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{4},y,-\frac{1}{4}$ (22) $2(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},\frac{1}{4},x$ (23) $4^-(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$ (24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},\frac{1}{4},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$			Reflection conditions
									h,k,l permutable
									General:
96	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl: $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl: $h+l=2n$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$			$h00$: $h=2n$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$			
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$			
									Special: as above, plus
48	i	2 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	hkl: $h=2n$
			$\frac{1}{4},x,\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x$	
48	h	. . 2	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$	no extra conditions
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$	
48	g	. . 2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$	no extra conditions
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
32	f	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
24	e	4 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24	d	2 . 2 2	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h=2n$
8	c	2 3 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$					hkl: $h=2n$
4	b	4 3 2	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						no extra conditions
4	a	4 3 2	$0,0,0$						no extra conditions

Symmetry of special projections

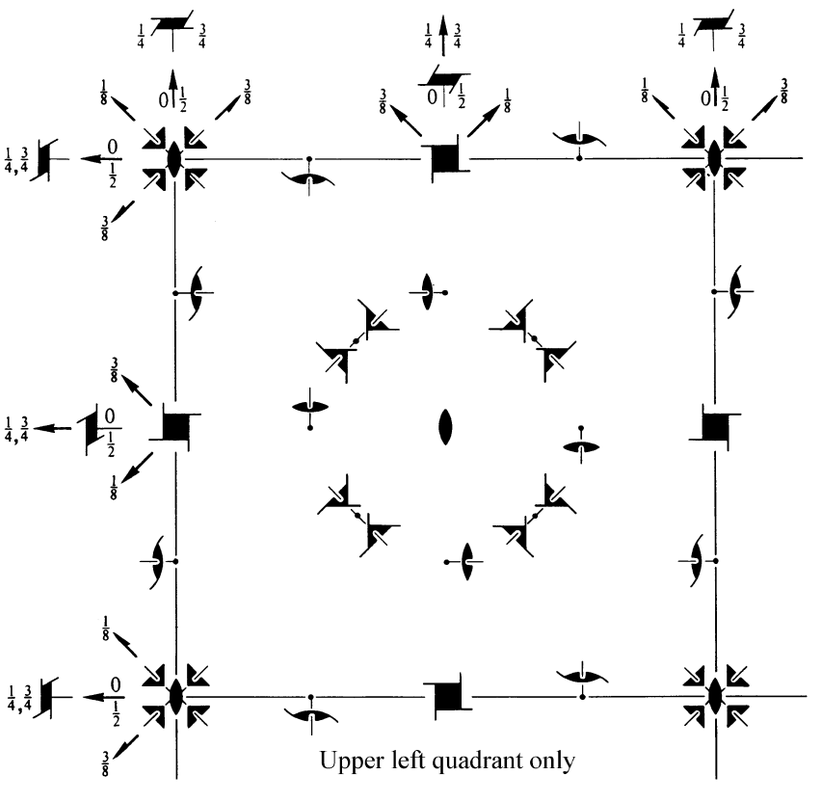
Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$F4_132$ O^4 432 Cubic

No. 210 $F4_132$ Patterson symmetry $Fm\bar{3}m$



Origin at 2 3

Asymmetric unit $0 \le x \le \frac{1}{2}$; $-\frac{1}{8} \le y \le \frac{1}{8}$; $-\frac{1}{8} \le z \le \frac{1}{8}$; $y \le \min(x, \frac{1}{2}-x)$; $-y \le z \le \min(x, \frac{1}{2}-x)$

Vertices $0,0,0$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{1}{8},-\frac{1}{8},\frac{1}{8}$
$\frac{1}{2},0,0$ $\frac{3}{8},\frac{1}{8},\frac{1}{8}$ $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{3}{8},-\frac{1}{8},\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) 3^+ x,x,x
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$
(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$
(14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{4})$ $0,\frac{3}{4},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y+\frac{1}{4},y$
(19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{3}{4}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{3}{4},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{3}{8},x$
(23) $4^-(0,\frac{3}{4},0)$ $\frac{1}{4},y,\frac{1}{2}$
(24) 2 $\bar{x}+\frac{1}{4},\frac{1}{8},x$

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Symmetry operations *(continued)*

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$ (2) $2\ 0,0,z$ (3) $2\ \frac{1}{4},y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)\ x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x-\frac{1}{3},x-\frac{1}{6},x$ (6) $3^+\ \bar{x}+\frac{1}{2},x,\bar{x}$ (7) $3^+\ x,\bar{x},\bar{x}$ (8) $3^+\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x-\frac{1}{6},x+\frac{1}{6},x$ (10) $3^-\ x+\frac{1}{2},\bar{x},\bar{x}$ (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) $3^-\ \bar{x},x,\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)\ x,x,\frac{1}{8}$ (14) $2(-\frac{1}{4},\frac{1}{4},0)\ x,\bar{x}+\frac{1}{2},\frac{3}{8}$ (15) $4^-(0,0,\frac{1}{4})\ \frac{1}{4},0,z$ (16) $4^+(0,0,\frac{3}{4})\ \frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{3}{4},0,0)\ x,\frac{1}{2},-\frac{1}{4}$ (18) $2(0,\frac{1}{2},\frac{1}{2})\ \frac{3}{8},y-\frac{1}{4},y$ (19) $2\ \frac{1}{8},y+\frac{3}{4},\bar{y}$ (20) $4^+(\frac{1}{4},0,0)\ x,0,\frac{1}{4}$
(21) $4^+(0,\frac{3}{4},0)\ \frac{1}{2},y,-\frac{1}{4}$ (22) $2(\frac{1}{4},0,\frac{1}{4})\ x,\frac{1}{8},x$ (23) $4^-(0,\frac{1}{4},0)\ 0,y,\frac{3}{4}$ (24) $2(-\frac{1}{4},0,\frac{1}{4})\ \bar{x}+\frac{1}{2},\frac{3}{8},x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$ (2) $2\ \frac{1}{4},\frac{1}{4},z$ (3) $2(0,\frac{1}{2},0)\ 0,y,\frac{1}{4}$ (4) $2\ x,0,0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{6},x-\frac{1}{6},x$ (6) $3^+\ \bar{x},x,\bar{x}$ (7) $3^+\ x+\frac{1}{2},\bar{x},\bar{x}$ (8) $3^+\ \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x-\frac{1}{6},x-\frac{1}{3},x$ (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) $3^-\ \bar{x},\bar{x},x$ (12) $3^-\ \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)\ x,x,\frac{1}{8}$ (14) $2(\frac{1}{4},-\frac{1}{4},0)\ x,\bar{x}+\frac{1}{2},\frac{3}{8}$ (15) $4^-(0,0,\frac{1}{4})\ \frac{3}{4},0,z$ (16) $4^+(0,0,\frac{3}{4})\ -\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)\ x,\frac{1}{4},0$ (18) $2(0,\frac{3}{4},\frac{3}{4})\ \frac{1}{8},y,y$ (19) $2(0,-\frac{1}{4},\frac{1}{4})\ \frac{3}{8},y+\frac{1}{2},\bar{y}$ (20) $4^+(\frac{3}{4},0,0)\ x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)\ \frac{1}{4},y,0$ (22) $2(\frac{1}{2},0,\frac{1}{2})\ x+\frac{1}{4},\frac{3}{8},x$ (23) $4^-(0,\frac{3}{4},0)\ -\frac{1}{4},y,\frac{1}{2}$ (24) $2\ \bar{x}+\frac{3}{4},\frac{1}{8},x$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2(0,0,\frac{1}{2})\ \frac{1}{4},0,z$ (3) $2\ 0,y,0$ (4) $2\ x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{6},x+\frac{1}{3},x$ (6) $3^+\ \bar{x},x+\frac{1}{2},\bar{x}$ (7) $3^+\ x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ (8) $3^+\ \bar{x},\bar{x},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\ x+\frac{1}{3},x+\frac{1}{6},x$ (10) $3^-\ x,\bar{x},\bar{x}$ (11) $3^-\ \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$ (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ x,x+\frac{1}{4},\frac{3}{8}$ (14) $2\ x,\bar{x}+\frac{3}{4},\frac{1}{8}$ (15) $4^-(0,0,\frac{3}{4})\ \frac{1}{2},-\frac{1}{4},z$ (16) $4^+(0,0,\frac{1}{4})\ 0,\frac{1}{4},z$
(17) $4^-(\frac{1}{4},0,0)\ x,\frac{3}{4},0$ (18) $2(0,\frac{1}{4},\frac{1}{4})\ \frac{1}{8},y,y$ (19) $2(0,\frac{1}{4},-\frac{1}{4})\ \frac{3}{8},y+\frac{1}{2},\bar{y}$ (20) $4^+(\frac{3}{4},0,0)\ x,-\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)\ \frac{1}{2},y,\frac{1}{4}$ (22) $2(\frac{3}{4},0,\frac{3}{4})\ x,\frac{1}{8},x$ (23) $4^-(0,\frac{1}{4},0)\ 0,y,\frac{1}{4}$ (24) $2(\frac{1}{4},0,-\frac{1}{4})\ \bar{x}+\frac{1}{2},\frac{3}{8},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							h,k,l permutable
							General:
96	h	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$	$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	hhl: $h+l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	$h00$: $h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
							Special: as above, plus
48	g	. . 2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{7}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{5}{8},\bar{y},y+\frac{1}{4}$	no extra conditions
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{7}{8},\bar{y}+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{8},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{5}{8},\bar{y}$	
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{7}{8}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{3}{8}$	$\bar{y},y+\frac{1}{4},\frac{5}{8}$	
48	f	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$0,x,0$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$0,0,x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	hkl: $h=2n+1$
			$\frac{3}{4},x+\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},x+\frac{3}{4}$	or $h+k+l=4n$
32	e	. 3 .	x,x,x	$\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$	$0kl$: $k+l=4n$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$	
16	d	. 3 2	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{7}{8}$	hkl: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	. 3 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{3}{8}$	
8	b	2 3 .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$			hkl: $h=2n+1$ or $h+k+l=4n$
8	a	2 3 .	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$			

Symmetry of special projections

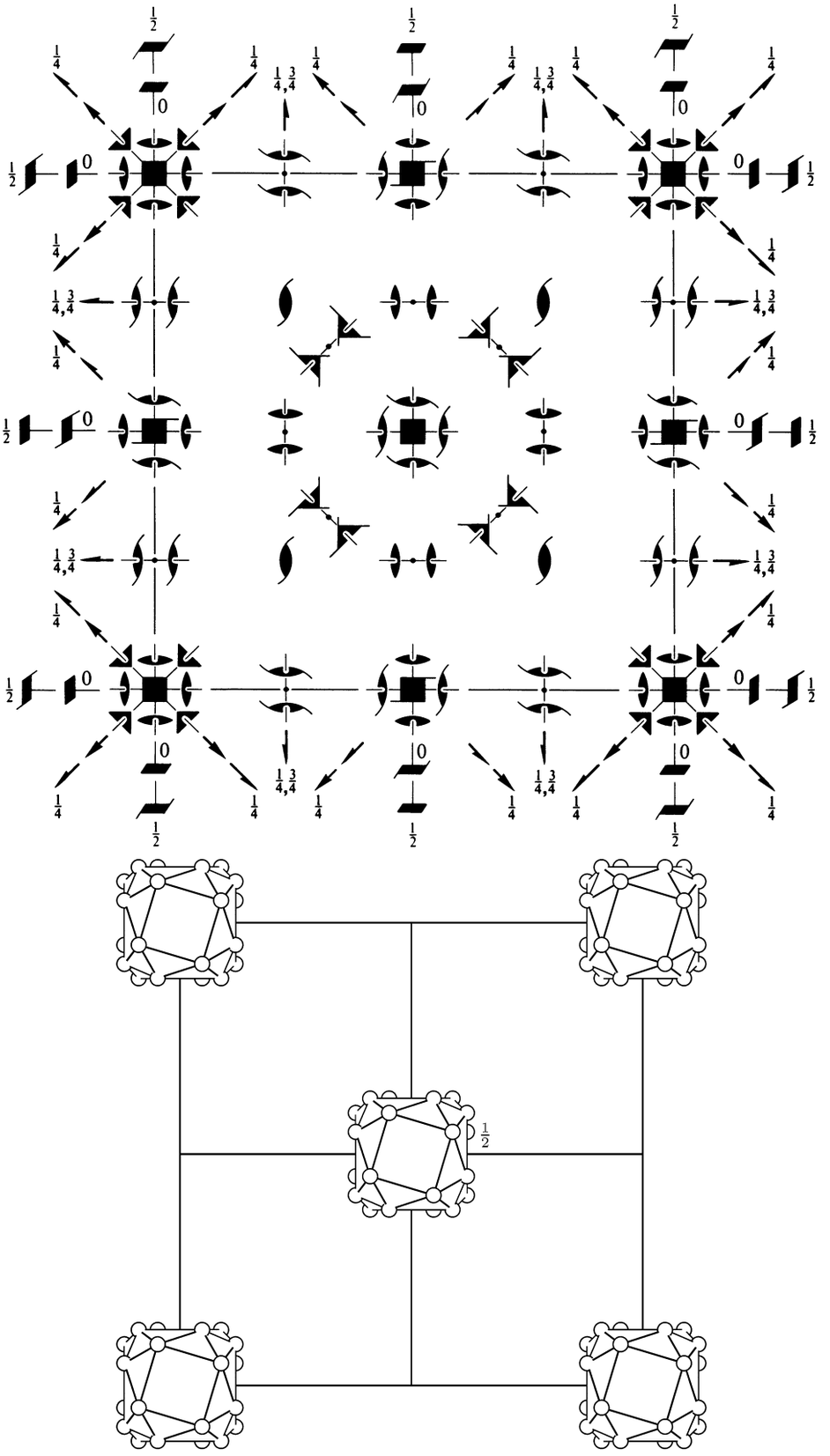
Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,\frac{1}{8}$

$I432$ O^5 432 Cubic

No. 211 $I432$ Patterson symmetry $Im\bar{3}m$



Origin at 432

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 x,x,0	(14) 2 $x,\bar{x}$,0	(15) 4^- 0,0,z	(16) 4^+ 0,0,z
(17) 4^- x,0,0	(18) 2 0,y,y	(19) 2 0,$y,\bar{y}$	(20) 4^+ x,0,0
(21) 4^+ 0,y,0	(22) 2 x,0,x	(23) 4^- 0,y,0	(24) 2 $\bar{x}$,0,x

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2}$,0,z	(16) $4^+(0,0,\frac{1}{2})$ 0,$\frac{1}{2}$,z
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,y$	(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0)$ x,0,$\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{2},y$,0	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0)$ 0,y,$\frac{1}{2}$	(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions h,k,l permutable
							General:
48	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$0kl$: $k+l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	hhl: $l=2n$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$	$h00$: $h=2n$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$	
							Special: as above, plus
24	i	. . 2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{3}{4},y,y+\frac{1}{2}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$	no extra conditions
			$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$	$y+\frac{1}{2},\frac{3}{4},y$	$y+\frac{1}{2},\frac{1}{4},\bar{y}$	
			$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y,y+\frac{1}{2},\frac{3}{4}$	$\bar{y},y+\frac{1}{2},\frac{1}{4}$	
24	h	. . 2	0,y,y	0,$\bar{y},y$	0,$y,\bar{y}$	0,$\bar{y},\bar{y}$	y,0,y	y,0,$\bar{y}$	no extra conditions
			$\bar{y}$,0,y	$\bar{y}$,0,$\bar{y}$	y,y,0	$\bar{y},y$,0	$y,\bar{y}$,0	$\bar{y},\bar{y}$,0	
24	g	2 . .	$x,\frac{1}{2}$,0	$\bar{x},\frac{1}{2}$,0	0,$x,\frac{1}{2}$	0,$\bar{x},\frac{1}{2}$	$\frac{1}{2}$,0,x	$\frac{1}{2}$,0,$\bar{x}$	no extra conditions
			$\frac{1}{2},x$,0	$\frac{1}{2},\bar{x}$,0	x,0,$\frac{1}{2}$	$\bar{x}$,0,$\frac{1}{2}$	0,$\frac{1}{2},\bar{x}$	0,$\frac{1}{2},x$	
16	f	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			no extra conditions
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$			
12	e	4 . .	x,0,0	$\bar{x}$,0,0	0,x,0	0,$\bar{x}$,0	0,0,x	0,0,$\bar{x}$	no extra conditions
12	d	2 . 2 2	$\frac{1}{4},\frac{1}{2}$,0	$\frac{3}{4},\frac{1}{2}$,0	0,$\frac{1}{4},\frac{1}{2}$	0,$\frac{3}{4},\frac{1}{2}$	$\frac{1}{2}$,0,$\frac{1}{4}$	$\frac{1}{2}$,0,$\frac{3}{4}$	no extra conditions
8	c	. 3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $k,l=2n$
6	b	4 2 . 2	0,$\frac{1}{2},\frac{1}{2}$	$\frac{1}{2}$,0,$\frac{1}{2}$	$\frac{1}{2},\frac{1}{2}$,0				no extra conditions
2	a	4 3 2	0,0,0						no extra conditions

Symmetry of special projections

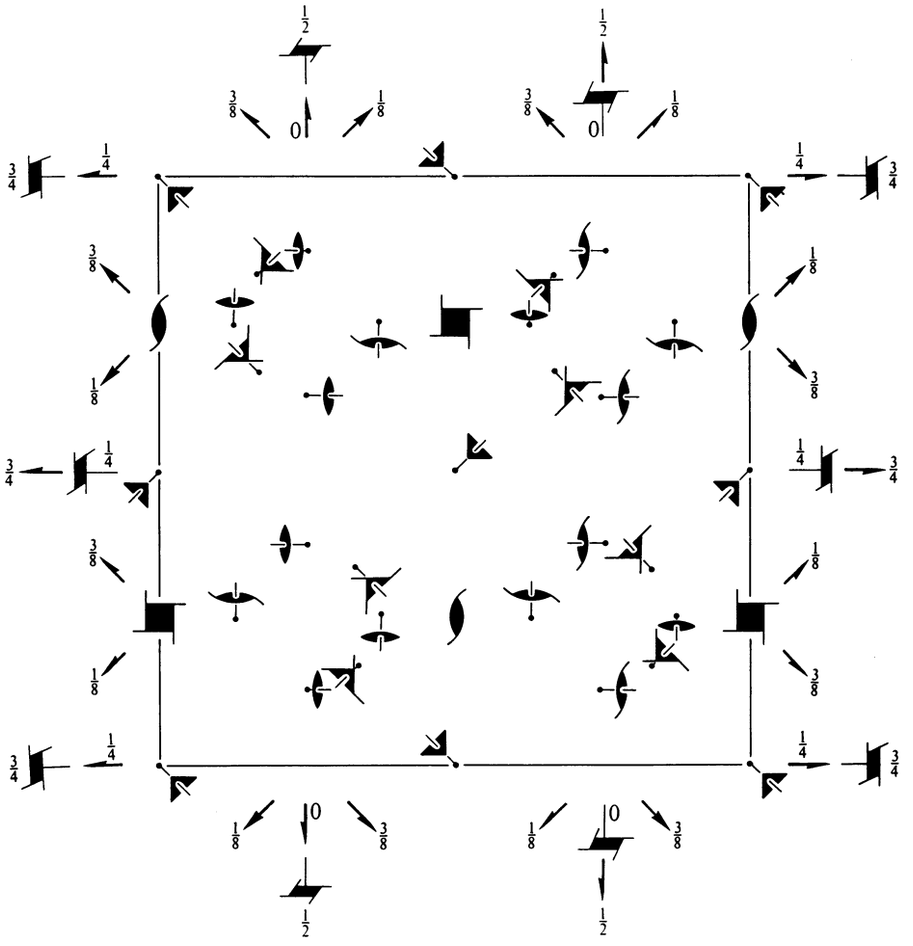
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

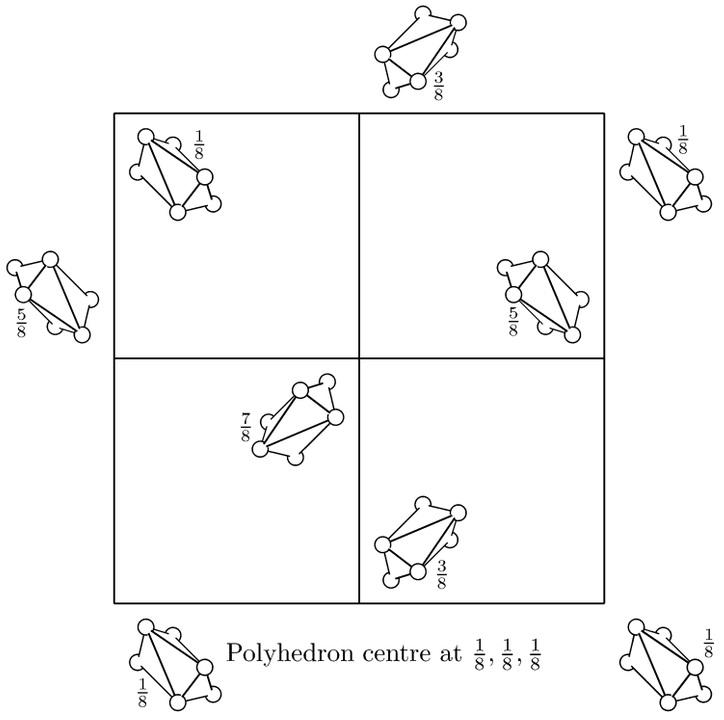
Along [111] $p3m1$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

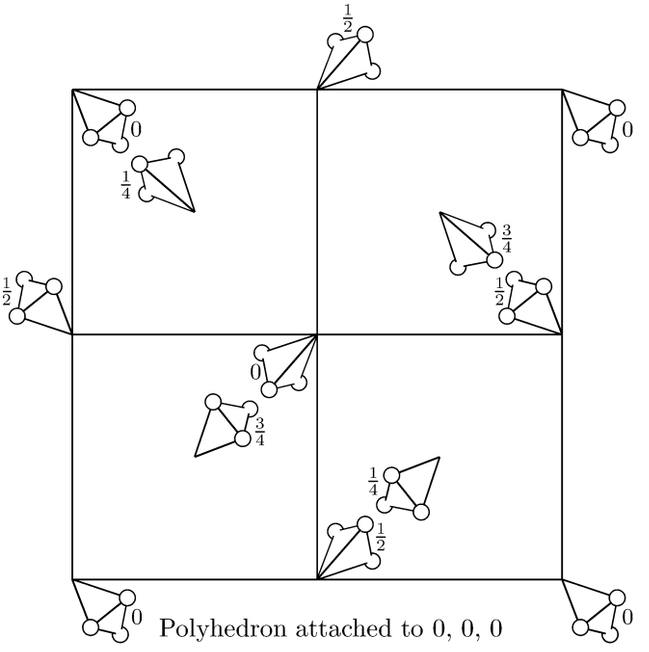
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P4_332$ O^6 432 Cubic

No. 212 $P4_332$ Patterson symmetry $Pm\bar{3}m$







Origin on 3[111] at midpoint of three non-intersecting pairs of parallel screw axes 4_3 and 2_1

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{3}{4}$; $-\frac{1}{2} \le z \le \frac{1}{4}$; $\max(-y, x-\frac{1}{2}) \le z \le \min(-y+\frac{1}{2}, 2x-y, 2y-x, y-2x+\frac{1}{2})$

Vertices $0,0,0$ $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$ $0,\frac{1}{2},-\frac{1}{2}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

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Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$	(14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$	(15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$	(16) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{4},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y-\frac{1}{4},y$	(19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$	(20) $4^+(\frac{3}{4},0,0)$ $x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,\frac{1}{4}$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{3}{8},x$	(23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{3}{4}$	(24) 2 $\bar{x}+\frac{1}{4},\frac{1}{8},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable
							General:
24	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00$: $h=4n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			(13) $y+\frac{1}{4},x+\frac{3}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{3}{4},\bar{x}+\frac{3}{4},z+\frac{1}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{1}{4},z+\frac{3}{4}$	
			(17) $x+\frac{1}{4},z+\frac{3}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{1}{4},y+\frac{3}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{3}{4},\bar{z}+\frac{3}{4},y+\frac{1}{4}$	
			(21) $z+\frac{1}{4},y+\frac{3}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{3}{4},\bar{y}+\frac{3}{4},x+\frac{1}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{1}{4},x+\frac{3}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
							Special: as above, plus
12	d	. . 2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$	no extra conditions
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$	$y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$	
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$	
8	c	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	$0kl$: $k=2n+1$
			$x+\frac{1}{4},x+\frac{3}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{3}{4},\bar{x}+\frac{3}{4},x+\frac{1}{4}$	$\bar{x}+\frac{3}{4},x+\frac{1}{4},x+\frac{3}{4}$	or $l=2n+1$
							or $k+l=4n$
4	b	. 3 2	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{7}{8},\frac{3}{8},\frac{1}{8}$	$\frac{3}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{3}{8}$	hkl: $h,k=2n+1$
4	a	. 3 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	or $h=2n+1$, $k=4n$ and $l=4n+2$
							or $h,k,l=4n+2$
							or $h,k,l=4n$

Symmetry of special projections

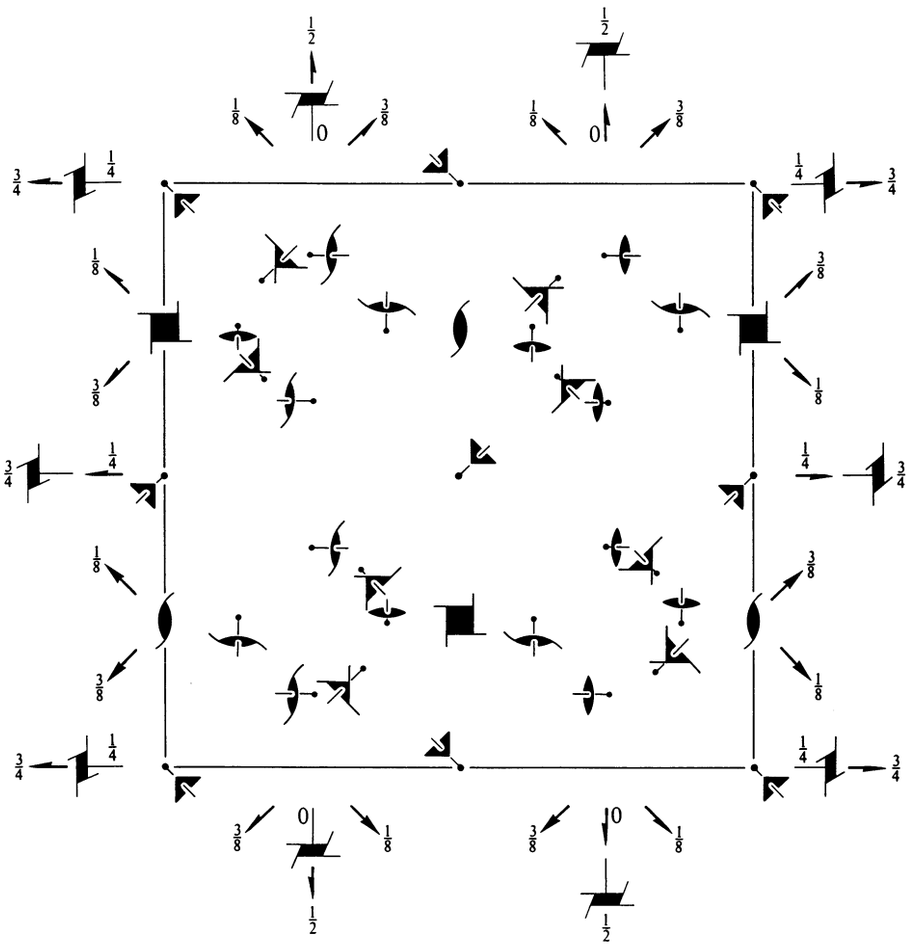
Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},\frac{1}{2},z$

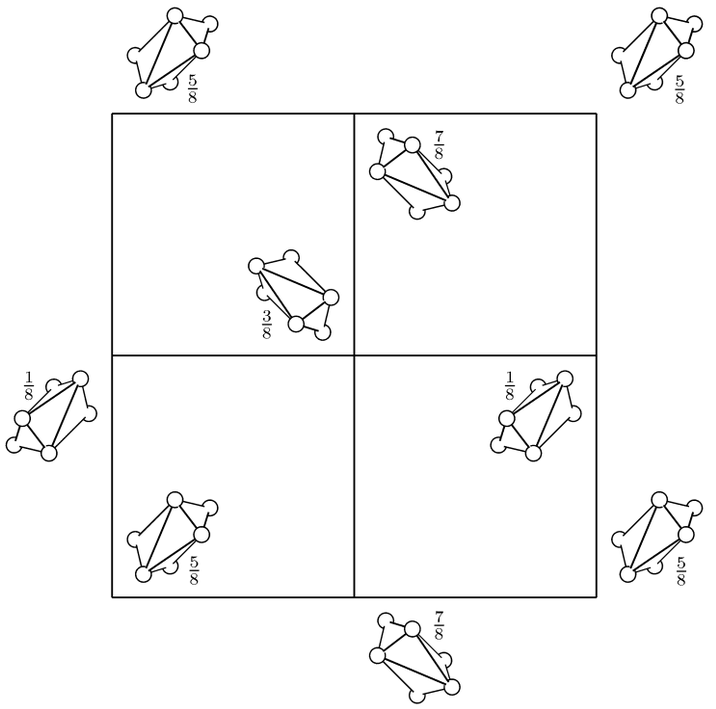
Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{3}{8}$

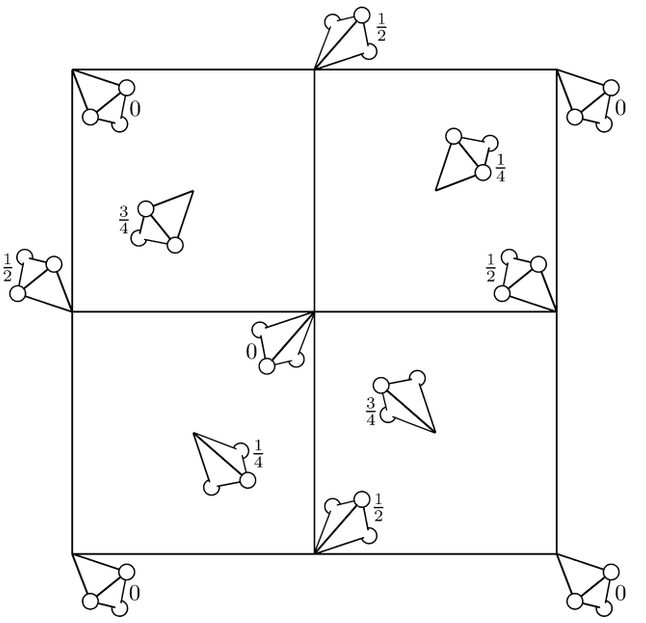
$P4_132$ O^7 432 Cubic

No. 213 $P4_132$ Patterson symmetry $Pm\bar{3}m$





Polyhedron centre at $\frac{3}{8},\frac{3}{8},\frac{3}{8}$



Polyhedron attached to 0, 0, 0

Origin on 3[111] at midpoint of three non-intersecting pairs of parallel screw axes 4_1 and 2_1

Asymmetric unit $-\frac{1}{4}\le x\le\frac{1}{2};\quad 0\le y\le\frac{3}{4};\quad 0\le z\le\frac{1}{2};\quad x\le y\le x+\frac{1}{2};\quad (y-x)/2\le z\le\min(y,(-4x-2y+3)/2,(3-2x-2y)/4)$

Vertices $0,0,0\quad \frac{1}{2},\frac{1}{2},0\quad \frac{1}{4},\frac{3}{4},\frac{1}{4}\quad -\frac{1}{4},\frac{1}{4},\frac{1}{4}\quad 0,\frac{1}{2},\frac{1}{2}\quad \frac{3}{8},\frac{3}{8},\frac{3}{8}$

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Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$	(14) 2 $x,\bar{x}+\frac{3}{4},\frac{3}{8}$	(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$	(16) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{4},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{8},y+\frac{1}{4},y$	(19) 2 $\frac{3}{8},y+\frac{3}{4},\bar{y}$	(20) $4^+(\frac{1}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{2},y,-\frac{1}{4}$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{1}{8},x$	(23) $4^-(0,\frac{3}{4},0)$ $0,y,\frac{1}{4}$	(24) 2 $\bar{x}+\frac{3}{4},\frac{3}{8},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable
							General:
24	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$h00$: $h=4n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$	
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$	
							Special: as above, plus
12	d	. . 2	$\frac{1}{8},y,y+\frac{1}{4}$	$\frac{3}{8},\bar{y},y+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	no extra conditions
			$y+\frac{1}{4},\frac{1}{8},y$	$y+\frac{3}{4},\frac{3}{8},\bar{y}$	$\bar{y}+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$\bar{y}+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$	
			$y,y+\frac{1}{4},\frac{1}{8}$	$\bar{y},y+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{5}{8}$	
8	c	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	$0kl$: $k=2n+1$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$	or $l=2n+1$
							or $k+l=4n$
4	b	. 3 2	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{1}{8}$	hkl: $h,k=2n+1$
4	a	. 3 2	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$\frac{1}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{5}{8}$	or $h=2n+1$, $k=4n$ and $l=4n+2$
							or $h,k,l=4n+2$
							or $h,k,l=4n$

Symmetry of special projections

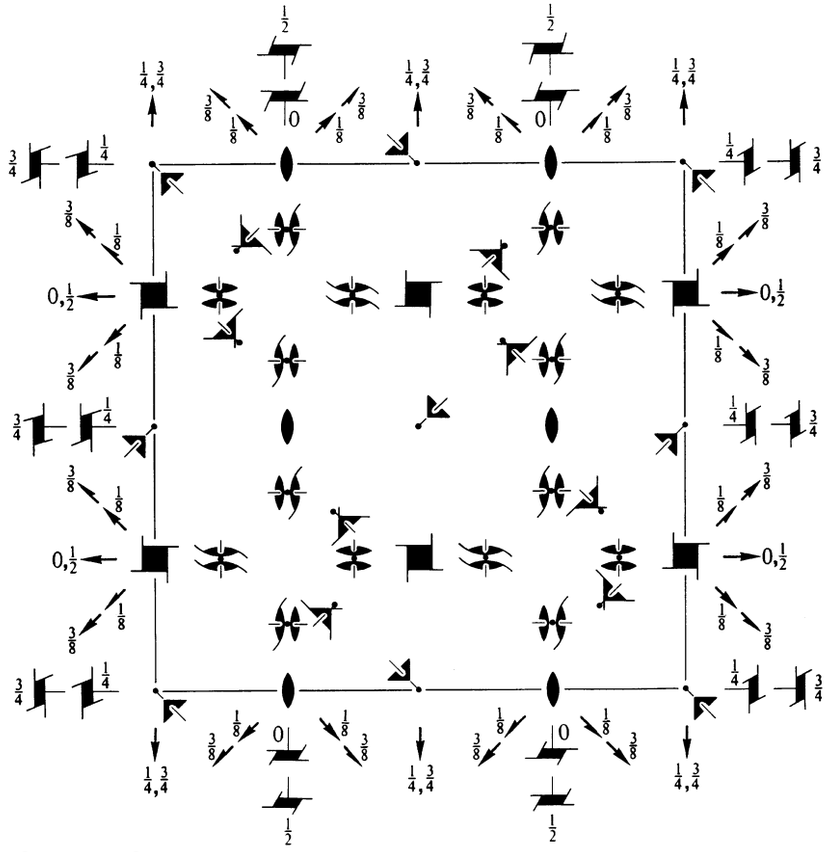
Along [001] $p4gm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{4},0,z$

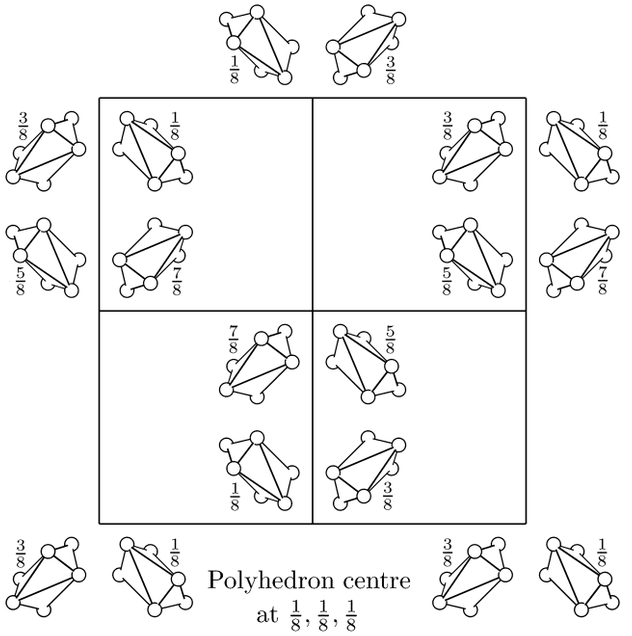
Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

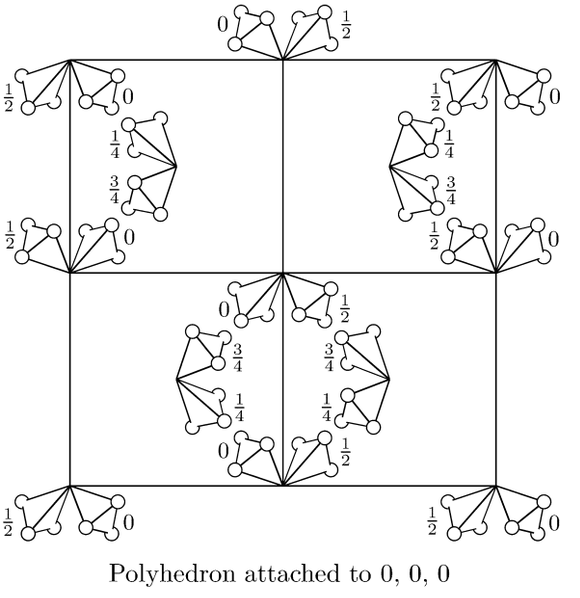
Along [110] $p2gm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{1}{8}$

$I4_132$ O^8 432 Cubic

No. 214 $I4_132$ Patterson symmetry $Im\bar{3}m$







Origin on 3[111] at midpoint of three non-intersecting pairs of parallel screw axes 4_1 and 4_3 and of three non-intersecting pairs of parallel 2 axes

Asymmetric unit $-\frac{3}{8}\le x\le\frac{1}{8}$; $-\frac{1}{8}\le y\le\frac{1}{8}$; $-\frac{1}{8}\le z\le\frac{3}{8}$; $\max(x,y,y-x-\frac{1}{8})\le z\le y+\frac{1}{4}$

Vertices $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},\frac{3}{8}$ $\frac{1}{8},-\frac{1}{8},\frac{1}{8}$ $-\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ $-\frac{3}{8},\frac{1}{8},\frac{3}{8}$ $-\frac{3}{8},-\frac{1}{8},\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$
(14) 2 $x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(16) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{4},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{8},y+\frac{1}{4},y$
(19) 2 $\frac{3}{8},y+\frac{3}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{2},y,-\frac{1}{4}$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{1}{8},x$
(23) $4^-(0,\frac{3}{4},0)$ $0,y,\frac{1}{4}$
(24) 2 $\bar{x}+\frac{3}{4},\frac{3}{8},x$

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Symmetry operations *(continued)*

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) $2\ \ 0,\frac{1}{4},z$ (3) $2\ \ \frac{1}{4},y,0$ (4) $2\ \ x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$ (6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ (7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,x$ (10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})\ \ x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})\ \ \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})\ \ \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\ \ x,x+\frac{1}{4},\frac{3}{8}$ (14) $2\ \ x,\bar{x}+\frac{1}{4},\frac{1}{8}$ (15) $4^-(0,0,\frac{1}{4})\ \ \frac{3}{4},0,z$ (16) $4^+(0,0,\frac{3}{4})\ \ \frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)\ \ x,\frac{3}{4},0$ (18) $2(0,\frac{1}{2},\frac{1}{2})\ \ \frac{3}{8},y-\frac{1}{4},y$ (19) $2\ \ \frac{1}{8},y+\frac{1}{4},\bar{y}$ (20) $4^+(\frac{3}{4},0,0)\ \ x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)\ \ \frac{1}{2},y,\frac{1}{4}$ (22) $2(\frac{1}{2},0,\frac{1}{2})\ \ x+\frac{1}{4},\frac{3}{8},x$ (23) $4^-(0,\frac{1}{4},0)\ \ 0,y,\frac{3}{4}$ (24) $2\ \ \bar{x}+\frac{1}{4},\frac{1}{8},x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$	Coordinates $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$	Reflection conditions
			h,k,l permutable General:
48 i 1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	hkl: $h+k+l=2n$
	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k+l=2n$
	(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	hhl: $l=2n$
	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$h00$: $h=4n$
	(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	
	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
	(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	
	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	
	(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	
	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$	
	(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	
	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$	
			Special: as above, plus
24 h . . 2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$ $\bar{y}+\frac{1}{4},\frac{1}{8},y$ $y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$ $\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$ $\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$	$\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$ $y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$ $y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$	$\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$ $y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$	no extra conditions
24 g . . 2	$\frac{1}{8},y,y+\frac{1}{4}$ $y+\frac{1}{4},\frac{1}{8},y$ $y,y+\frac{1}{4},\frac{1}{8}$	$\frac{3}{8},\bar{y},y+\frac{3}{4}$ $y+\frac{3}{4},\frac{3}{8},\bar{y}$ $\bar{y},y+\frac{3}{4},\frac{3}{8}$	$\frac{7}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$ $\bar{y}+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$ $y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{7}{8}$	$\frac{5}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$ $\bar{y}+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{5}{8}$	no extra conditions
24 f 2 . .	$x,0,\frac{1}{4}$ $\frac{3}{4},x+\frac{1}{4},0$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$ $\frac{3}{4},\bar{x}+\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},x,0$ $x+\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$ $\bar{x}+\frac{1}{4},0,\frac{1}{4}$	$0,\frac{1}{4},x$ $0,\frac{1}{4},\bar{x}+\frac{1}{4}$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{4},x+\frac{3}{4}$	hkl: $h=2n+1$ or $h=4n$ hhl: $h=2n+1$ or $h+k+l=4n$
16 e . 3 .	x,x,x $x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$ $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$ $\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$	$0kl$: $k=2n+1$ or $k+l=4n$
12 d 2 . 2 2	$\frac{5}{8},0,\frac{1}{4}$	$\frac{7}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{5}{8},0$	$\frac{3}{4},\frac{7}{8},0$	$0,\frac{1}{4},\frac{5}{8}$	$0,\frac{3}{4},\frac{7}{8}$	hkl: $h,k=2n$, $h+k+l=4n$ or $h,k=2n+1$, $l=4n+2$ or $h=8n$, $k=8n+4$ and $h+k+l=4n+2$ or $h,k=8n+1$, $l=4n$ or $h=8n+1$ and $k=8n-1$, $l=4n$ or $h,k=8n+3$, $l=4n$ or $h=8n+3$ and $k=8n-3$, $l=4n$
12 c 2 . 2 2	$\frac{1}{8},0,\frac{1}{4}$	$\frac{3}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{8},0$	$\frac{3}{4},\frac{3}{8},0$	$0,\frac{1}{4},\frac{1}{8}$	$0,\frac{3}{4},\frac{3}{8}$	
8 b . 3 2	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{1}{8}$	hkl: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
8 a . 3 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	

Symmetry of special projections

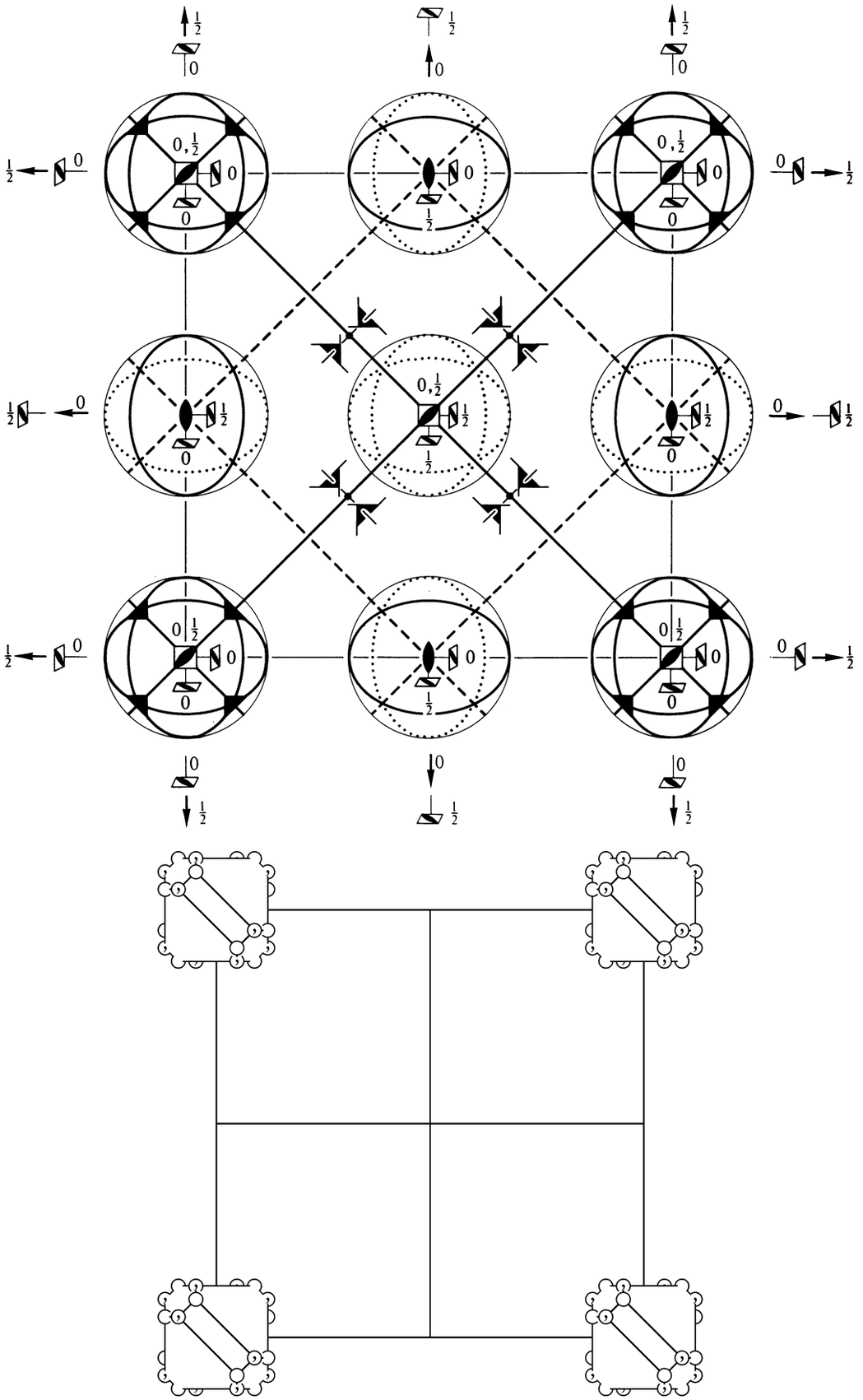
Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},0,z$

Along [111] $p3m1$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{1}{8}$

$P\bar{4}3m$ T_d^1 $\bar{4}3m$ Cubic

No. 215 $P\bar{4}3m$ Patterson symmetry $Pm\bar{3}m$



Origin at $\bar{4}3m$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{2};\quad y \le \min(x, 1-x);\quad z \le y$

Vertices $0,0,0\quad 1,0,0\quad \frac{1}{2},\frac{1}{2},0\quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) m x,x,z	(14) m $x,\bar{x},z$	(15) $\bar{4}^+$ $0,0,z;$ $0,0,0$	(16) $\bar{4}^-$ $0,0,z;$ $0,0,0$
(17) m x,y,y	(18) $\bar{4}^+$ $x,0,0;$ $0,0,0$	(19) $\bar{4}^-$ $x,0,0;$ $0,0,0$	(20) m $x,y,\bar{y}$
(21) m x,y,x	(22) $\bar{4}^-$ $0,y,0;$ $0,0,0$	(23) m $\bar{x},y,x$	(24) $\bar{4}^+$ $0,y,0;$ $0,0,0$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable
							General:
24	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	no conditions
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$	
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$	
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$	
							Special: no extra conditions
12	i	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x $z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$ $\bar{x},\bar{z},x$
12	h	$2..$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$ $\frac{1}{2},0,\bar{x}$
			$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\frac{1}{2},x$ $0,\frac{1}{2},\bar{x}$
6	g	$2.mm$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$ $\frac{1}{2},\frac{1}{2},\bar{x}$
6	f	$2.mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$ $0,0,\bar{x}$
4	e	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$	
3	d	$\bar{4}2.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$		
3	c	$\bar{4}2.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		
1	b	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	a	$\bar{4}3m$	$0,0,0$				

Symmetry of special projections

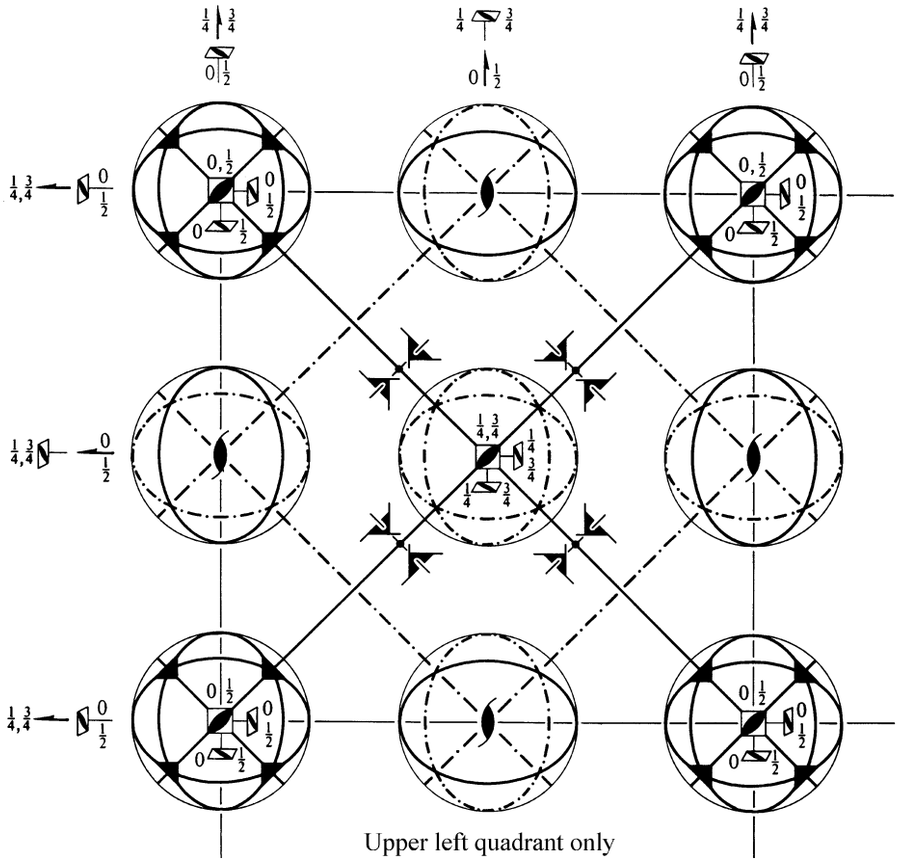
Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

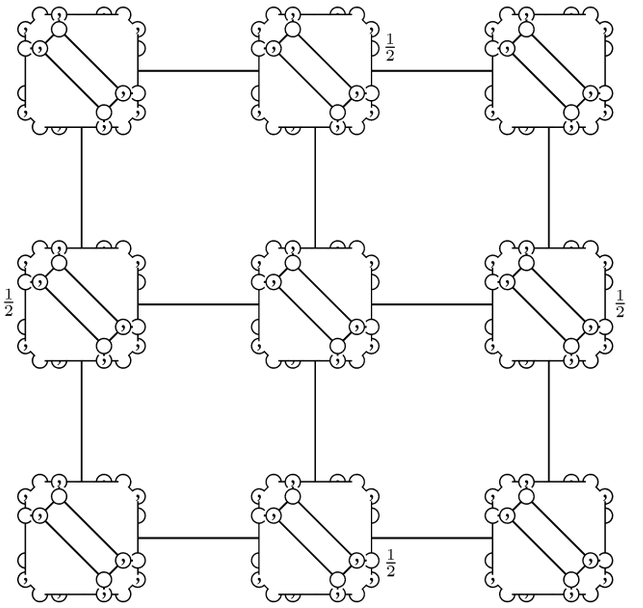
Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$F\bar{4}3m$ T_d^2 $\bar{4}3m$ Cubic

No. 216 $F\bar{4}3m$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Origin at $\bar{4}\,3\,m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2} - x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) m x,x,z	(14) m $x,\bar{x},z$	(15) $\bar{4}^+$ $0,0,z$; $0,0,0$	(16) $\bar{4}^-$ $0,0,z$; $0,0,0$
(17) m x,y,y	(18) $\bar{4}^+$ $x,0,0$; $0,0,0$	(19) $\bar{4}^-$ $x,0,0$; $0,0,0$	(20) m $x,y,\bar{y}$
(21) m x,y,x	(22) $\bar{4}^-$ $0,y,0$; $0,0,0$	(23) m $\bar{x},y,x$	(24) $\bar{4}^+$ $0,y,0$; $0,0,0$

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Symmetry operations *(continued)*

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$
(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$
(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$
(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$
(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x-\frac{1}{4},x,z$
(14) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$
(15) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(16) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(17) $g(0,\frac{1}{2},\frac{1}{2})$ x,y,y
(18) $\bar{4}^+$ $x,\frac{1}{2},0$; $0,\frac{1}{2},0$
(19) $\bar{4}^-$ $x,0,\frac{1}{2}$; $0,0,\frac{1}{2}$
(20) m $x,y+\frac{1}{2},\bar{y}$
(21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x-\frac{1}{4},y,x$
(22) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(23) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(24) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(3) 2 $\frac{1}{4},y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$
(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},x,z$
(14) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$
(15) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(16) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$
(18) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(19) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(20) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{2},0,\frac{1}{2})$ x,y,x
(22) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},0,0$
(23) m $\bar{x}+\frac{1}{2},y,x$
(24) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,0,\frac{1}{2}$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$
(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$
(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z
(14) m $x+\frac{1}{2},\bar{x},z$
(15) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,0$
(16) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},0$
(17) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$
(18) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(19) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(20) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x+\frac{1}{4},y,x$
(22) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(23) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(24) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							h,k,l permutable
							General:
96	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl: $h+k,h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	hhl: $h+l=2n$
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$	$h00$: $h=2n$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$	
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$	
							Special: no extra conditions
48	h	$..m$	x,x,z $\bar{z},\bar{x},x$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$	$\bar{x},x,\bar{z}$ x,z,x	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$	z,x,x $x,\bar{z},\bar{x}$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$
24	g	$2\,.\,mm$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$
24	f	$2\,.\,mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
16	e	$.\,3\,m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
4	d	$\bar{4}\,3\,m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					
4	c	$\bar{4}\,3\,m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$					
4	b	$\bar{4}\,3\,m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
4	a	$\bar{4}\,3\,m$	$0,0,0$					

Symmetry of special projections

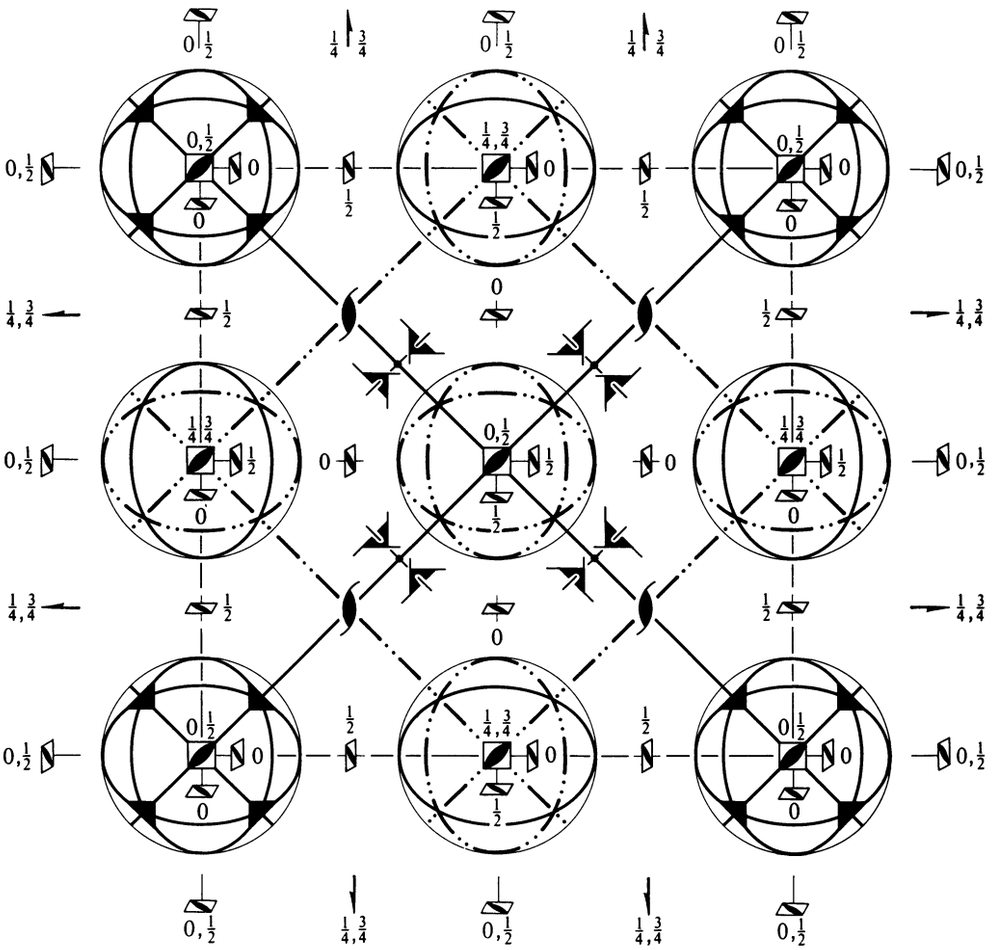
Along [001] $p4mm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

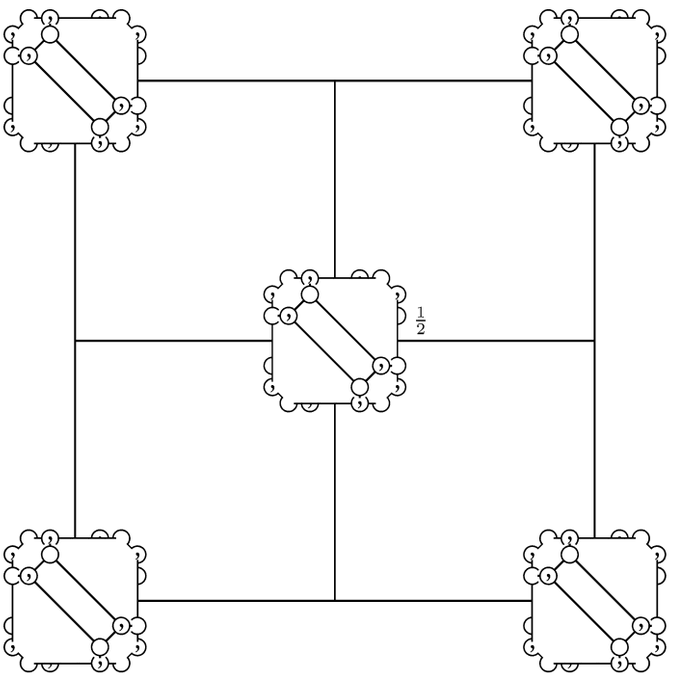
Along [111] $p31m$
$\mathbf{a}'=\frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

$I\bar{4}3m$ T_d^3 $\bar{4}3m$ Cubic

No. 217 $I\bar{4}3m$ Patterson symmetry $Im\bar{3}m$





Origin at $\bar{4}3m$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) m x,x,z	(14) m $x,\bar{x},z$	(15) $\bar{4}^+$ 0,0,z; 0,0,0	(16) $\bar{4}^-$ 0,0,z; 0,0,0
(17) m x,y,y	(18) $\bar{4}^+$ x,0,0; 0,0,0	(19) $\bar{4}^-$ x,0,0; 0,0,0	(20) m $x,y,\bar{y}$
(21) m x,y,x	(22) $\bar{4}^-$ 0,y,0; 0,0,0	(23) m $\bar{x},y,x$	(24) $\bar{4}^+$ 0,y,0; 0,0,0

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(14) c $x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{2}$,0,z; $\frac{1}{2}$,0,$\frac{1}{4}$	(16) $\bar{4}^-$ 0,$\frac{1}{2}$,z; 0,$\frac{1}{2}$,$\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(18) $\bar{4}^+$ x,$\frac{1}{2}$,0; $\frac{1}{4}$,$\frac{1}{2}$,0	(19) $\bar{4}^-$ x,0,$\frac{1}{2}$; $\frac{1}{4}$,0,$\frac{1}{2}$	(20) a $x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(22) $\bar{4}^-$ $\frac{1}{2}$,y,0; $\frac{1}{2}$,$\frac{1}{4}$,0	(23) b $\bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^+$ 0,y,$\frac{1}{2}$; 0,$\frac{1}{4}$,$\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
							h,k,l permutable
							General:
48	h	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$0kl$: $k+l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	hhl: $l=2n$
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$	$h00$: $h=2n$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$	
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$	
							Special: no extra conditions
24	g	. . m	x,x,z $\bar{z},\bar{x},x$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$	$\bar{x},x,\bar{z}$ x,z,x	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$	z,x,x $x,\bar{z},\bar{x}$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$
24	f	2 . .	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},x$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},\bar{x}$
12	e	2 . mm	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
12	d	$\bar{4}$ . .	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$
8	c	. 3 m	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
6	b	$\bar{4}$ 2 . m	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
2	a	$\bar{4}$ 3 m	0,0,0					

Symmetry of special projections

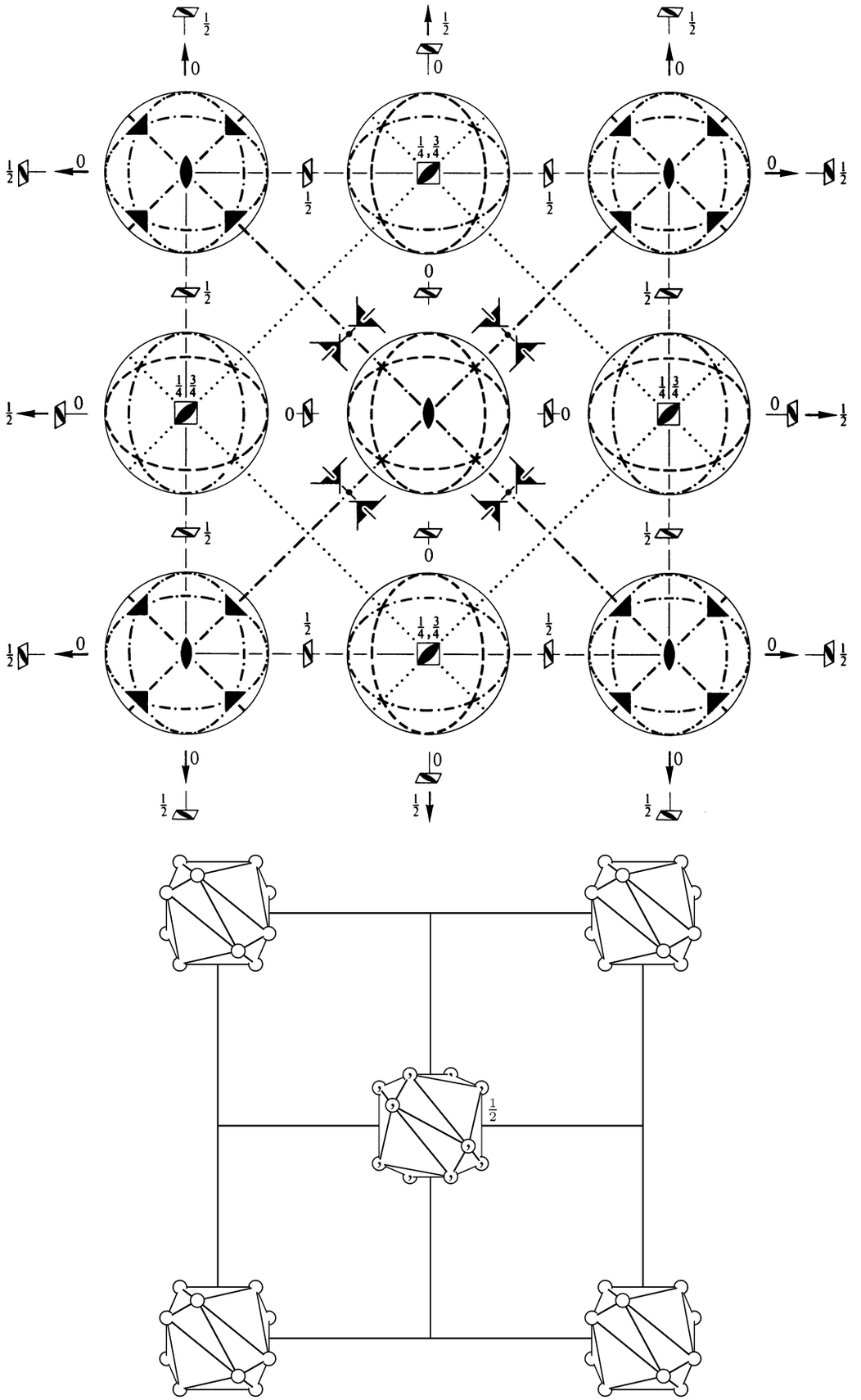
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$P\bar{4}3n$ T_d^4 $\bar{4}3m$ Cubic

No. 218 $P\bar{4}3n$ Patterson symmetry $Pm\bar{3}m$



Origin at 2 3

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}; \quad z \le \min(x,y)$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad 0,\frac{1}{2},0 \quad \frac{1}{2},\frac{1}{2},\frac{1}{2}$

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Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 2 $0,y,0$	(4) 2 $x,0,0$
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(14) c $x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(16) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(18) $\bar{4}^+$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$	(19) $\bar{4}^-$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$	(20) a $x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(22) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$	(23) b $\bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable
							General:
24	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hhl: $l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	$h00$: $h=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	
							Special: as above, plus
12	h	2 . .	$x,0,\frac{1}{2}$ $\frac{1}{2},x+\frac{1}{2},0$	$\bar{x},0,\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x,0$ $x+\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\bar{x},0$ $\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},x$ $0,\frac{1}{2},x+\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$ $0,\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl: $h=2n$
12	g	2 . .	$x,\frac{1}{2},0$ $0,x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$ $0,\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,x$ $\frac{1}{2},0,x+\frac{1}{2}$	$\frac{1}{2},0,\bar{x}$ $\frac{1}{2},0,\bar{x}+\frac{1}{2}$	hkl: $h=2n$
12	f	2 . .	$x,0,0$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,0$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\bar{x},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,x$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	$0,0,\bar{x}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl: $h+k+l=2n$
8	e	. 3 .	x,x,x $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{x},x$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},x,\bar{x}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x,\bar{x},\bar{x}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$			hkl: $h+k+l=2n$
6	d	$\bar{4}$ . .	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl: $h+k+l=2n$ or $h=2n+1$, $k=4n$ and $l=4n+2$
6	c	$\bar{4}$ . .	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	
6	b	2 2 2 . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl: $h+k+l=2n$
2	a	2 3 .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl: $h+k+l=2n$

Symmetry of special projections

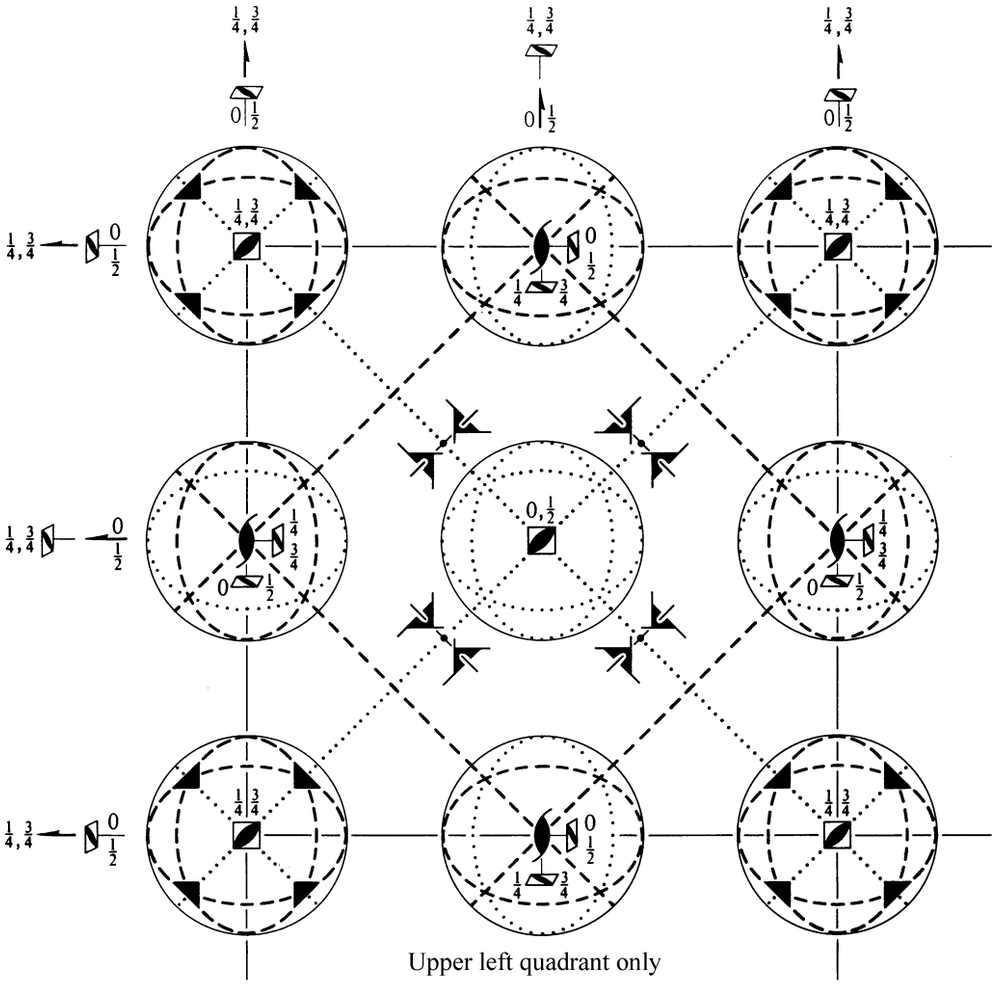
Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $\frac{1}{2},0,z$

Along [111] $p31m$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

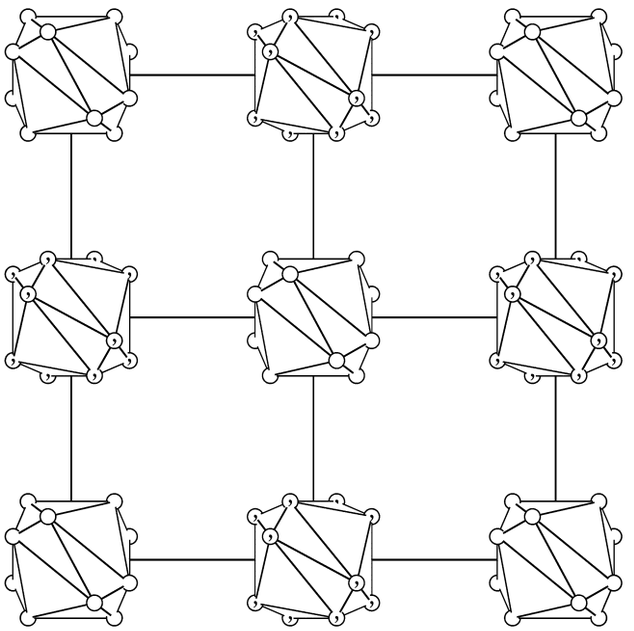
Along [110] $p1m1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$F\bar{4}3c$ T_d^5 $\bar{4}3m$ Cubic

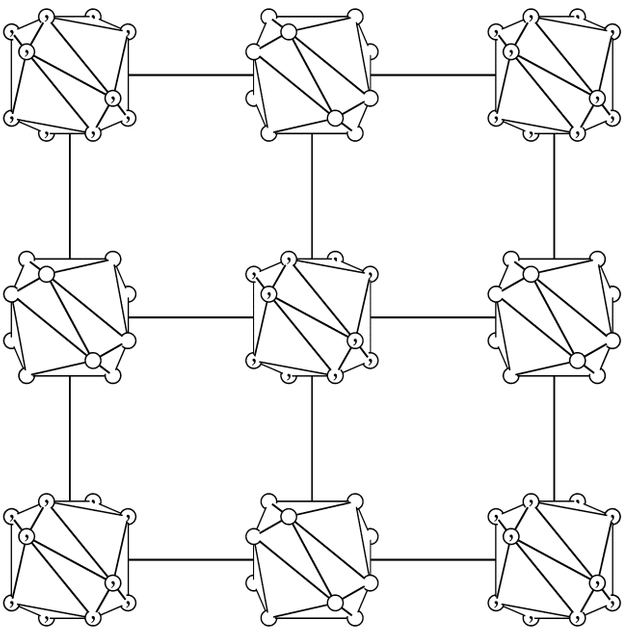
No. 219 $F\bar{4}3c$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only



Lower half of unit cell, all polyhedra at height 0



Upper half of unit cell, all polyhedra at height $\frac{1}{2}$

Origin at 2 3

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2}-x)$; $-y \le z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

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Symmetry operations

For $(0,0,0)+$ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(14) c $x+\frac{1}{2},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$	(16) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(17) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(18) $\bar{4}^+$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$	(19) $\bar{4}^-$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$	(20) a $x,y+\frac{1}{2},\bar{y}$
(21) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x	(22) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$	(23) b $\bar{x}+\frac{1}{2},y,x$	(24) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$	(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$	(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$	(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$	(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$	(14) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$	(16) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$
(17) a x,y,y	(18) $\bar{4}^+$ $x,0,0$; $\frac{1}{4},0,0$	(19) $\bar{4}^-$ $x,0,0$; $\frac{1}{4},0,0$	(20) a $x,y,\bar{y}$
(21) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$	(22) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},0,-\frac{1}{4}$	(23) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) 2 $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$	(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$	(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$	(14) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$	(15) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$	(16) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$
(17) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$	(18) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}$; $0,\frac{1}{4},-\frac{1}{4}$	(19) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$	(20) $g(0,\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(21) b x,y,x	(22) $\bar{4}^-$ $0,y,0$; $0,\frac{1}{4},0$	(23) b $\bar{x},y,x$	(24) $\bar{4}^+$ $0,y,0$; $0,\frac{1}{4},0$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) 2 $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$	(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$	(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$	(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$	(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$	(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) c x,x,z	(14) c $x,\bar{x},z$	(15) $\bar{4}^+$ 0,0,z; 0,0,$\frac{1}{4}$	(16) $\bar{4}^-$ 0,0,z; 0,0,$\frac{1}{4}$
(17) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$	(18) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$	(19) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}$; $0,-\frac{1}{4},\frac{1}{4}$	(20) $g(0,-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(21) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$	(22) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$	(23) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$	(24) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},0,\frac{1}{4}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
					h,k,l permutable
					General:
96 h 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl: $h+k=2n$ and $h+l,k+l=2n$
	(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	
	(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	$0kl$: $k,l=2n$
	(13) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	hhl: $h,l=2n$
	(17) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	$h00$: $h=2n$
	(21) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	
					Special: as above, plus
48 g 2 . .	$x,\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},x,\frac{1}{4}$ $x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$ $\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$ $\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{x}$ $\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl: $h=2n$
48 f 2 . .	$x,0,0$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},0,0$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x,0$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\bar{x},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,x$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	$0,0,\bar{x}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl: $h=2n$
32 e . 3 .	x,x,x $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{x},x$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},x,\bar{x}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x,\bar{x},\bar{x}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$			hkl: $h=2n$
24 d $\bar{4}$ . .	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$	$0,\frac{1}{4},0$	$0,\frac{3}{4},0$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$	hkl: $h=2n$
24 c $\bar{4}$ . .	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h=2n$
8 b 2 3 .	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl: $h=2n$
8 a 2 3 .	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl: $h=2n$

Symmetry of special projections

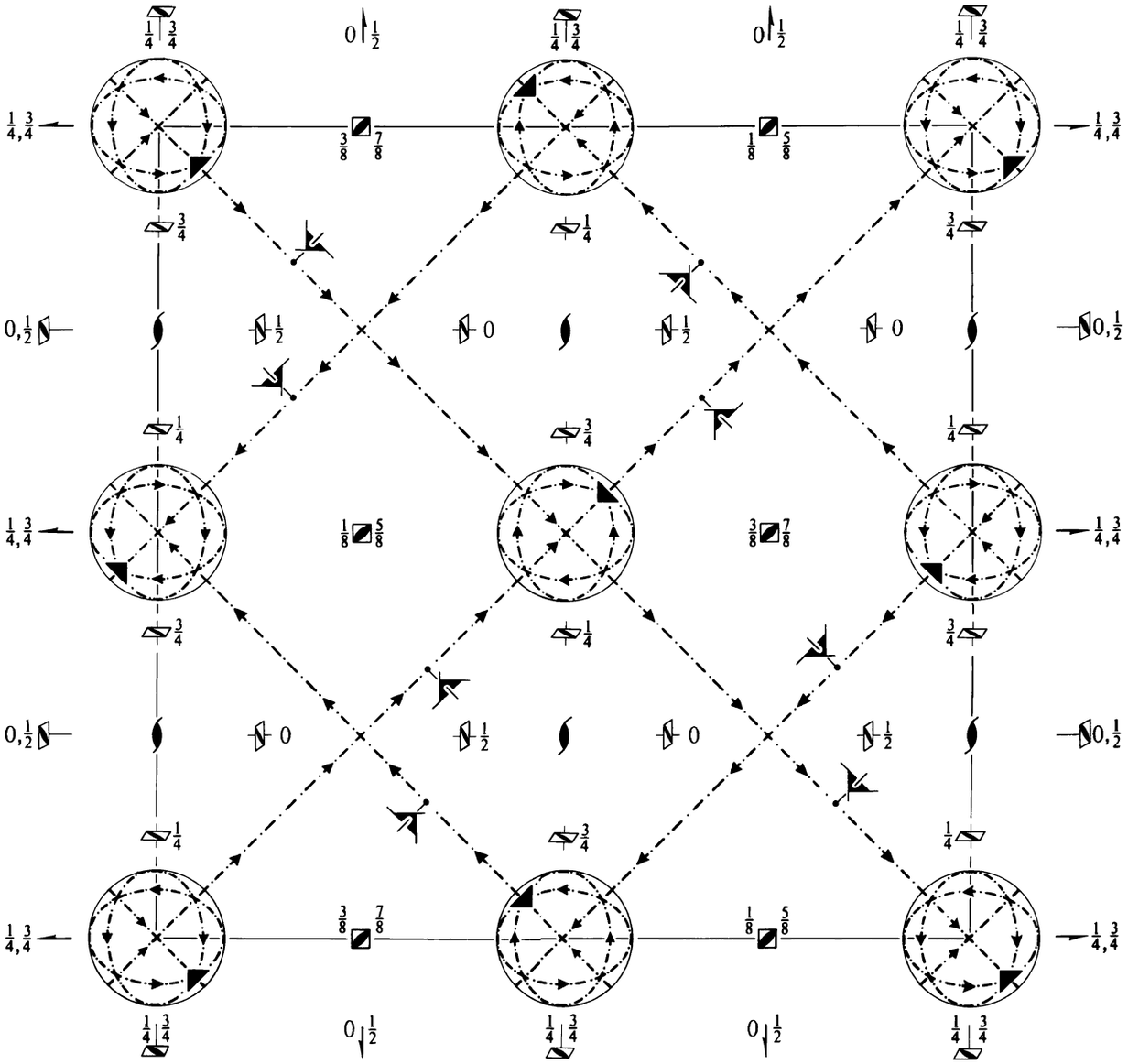
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

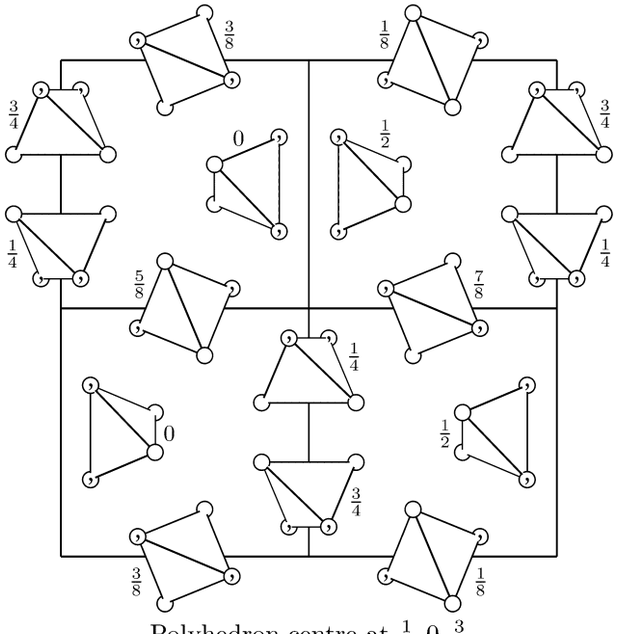
Along [111] $p31m$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p1m1$
$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

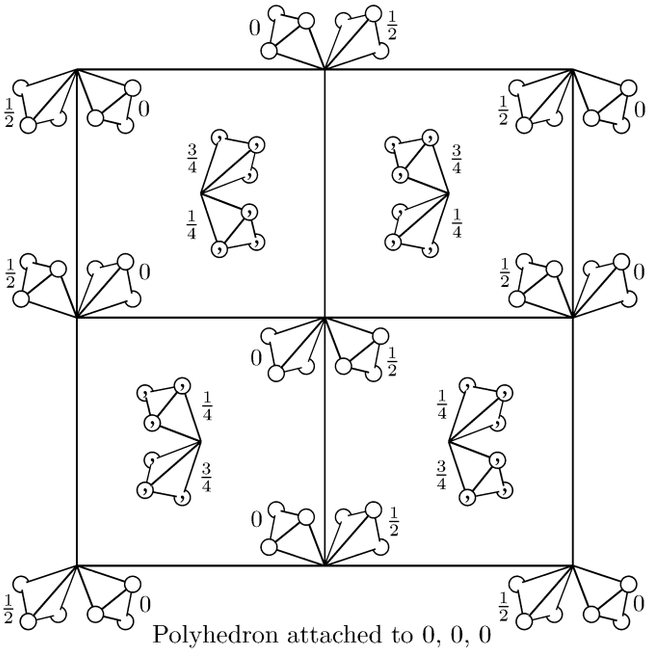
$I\bar{4}3d$ T_d^6 $\bar{4}3m$ Cubic

No. 220 $I\bar{4}3d$ Patterson symmetry $Im\bar{3}m$





Polyhedron centre at $\frac{1}{8}, 0, \frac{3}{4}$



Polyhedron attached to 0, 0, 0

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Origin on 3[111] at midpoint of three non-intersecting pairs of parallel $\bar{4}$ axes and of three non-intersecting pairs of parallel 2_1 axes

Asymmetric unit $\frac{1}{4} \le x \le \frac{1}{2}$; $\frac{1}{4} \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $z \le \min(x,y)$

Vertices $\frac{1}{4},\frac{1}{4},0$ $\frac{1}{2},\frac{1}{4},0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{2},\frac{1}{4},\frac{1}{4}$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{4},\frac{1}{2},\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x (6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$ (7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$ (8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x (10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,x,z (14) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$ (15) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$ (16) $\bar{4}^-$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
(17) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,y,y (18) $\bar{4}^+$ $x,\frac{1}{2},-\frac{1}{4}$; $\frac{3}{8},\frac{1}{2},-\frac{1}{4}$ (19) $\bar{4}^-$ $x,0,\frac{3}{4}$; $\frac{1}{8},0,\frac{3}{4}$ (20) $d(\frac{3}{4},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$
(21) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,y,x (22) $\bar{4}^-$ $\frac{3}{4},y,0$; $\frac{3}{4},\frac{1}{8},0$ (23) $d(\frac{1}{4},\frac{3}{4},-\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$ (24) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{2}$; $-\frac{1}{4},\frac{3}{8},\frac{1}{2}$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ (2) 2 $0,\frac{1}{4},z$ (3) 2 $\frac{1}{4},y,0$ (4) 2 $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x (6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$ (7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x (10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$ (11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$ (12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,x,z (14) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$ (15) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$ (16) $\bar{4}^-$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
(17) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,y,y (18) $\bar{4}^+$ $x,\frac{1}{2},\frac{1}{4}$; $\frac{1}{8},\frac{1}{2},\frac{1}{4}$ (19) $\bar{4}^-$ $x,0,\frac{1}{4}$; $\frac{3}{8},0,\frac{1}{4}$ (20) $d(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$
(21) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,y,x (22) $\bar{4}^-$ $\frac{1}{4},y,0$; $\frac{1}{4},\frac{3}{8},0$ (23) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$ (24) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{2}$; $\frac{1}{4},\frac{1}{8},\frac{1}{2}$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+	Coordinates $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			Reflection conditions
							h,k,l permutable
							General:
48	e	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	hhl: $2h+l=4n$
			(13) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(15) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	$h00$: $h=4n$
			(17) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	(20) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	
			(21) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$	(22) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	
							Special: as above, plus
24	d	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	hkl: $h=2n+1$
			$\frac{1}{4},x+\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\bar{x}+\frac{3}{4},0$	$x+\frac{1}{4},\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{3}{4},0,\frac{1}{4}$	or $h=4n$
			$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$			
			$\frac{1}{2},\frac{1}{4},x+\frac{1}{4}$	$0,\frac{1}{4},\bar{x}+\frac{3}{4}$			
16	c	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	hkl: $h=2n+1$
			$x+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$x+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},\bar{x}+\frac{1}{4}$	or $h+k+l=4n$
12	b	$\bar{4}$ . .	$\frac{7}{8},0,\frac{1}{4}$	$\frac{5}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{7}{8},0$	$\frac{3}{4},\frac{5}{8},0$	$0,\frac{1}{4},\frac{7}{8}$ $0,\frac{3}{4},\frac{5}{8}$	hkl: $h,k=2n$, $h+k+l=4n$
12	a	$\bar{4}$ . .	$\frac{3}{8},0,\frac{1}{4}$	$\frac{1}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{3}{8},0$	$\frac{3}{4},\frac{1}{8},0$	$0,\frac{1}{4},\frac{3}{8}$ $0,\frac{3}{4},\frac{1}{8}$	or $h,k=2n+1$, $l=4n+2$
								or $h=8n$, $k=8n+4$ and $h+k+l=4n+2$
								or $h=8n+1$ and $k=8n+3$, $l=4n$
								or $h=8n+1$ and $k=8n+5$, $l=4n$
								or $h=8n+7$ and $k=8n+3$, $l=4n$
								or $h=8n+7$ and $k=8n+5$, $l=4n$

Symmetry of special projections

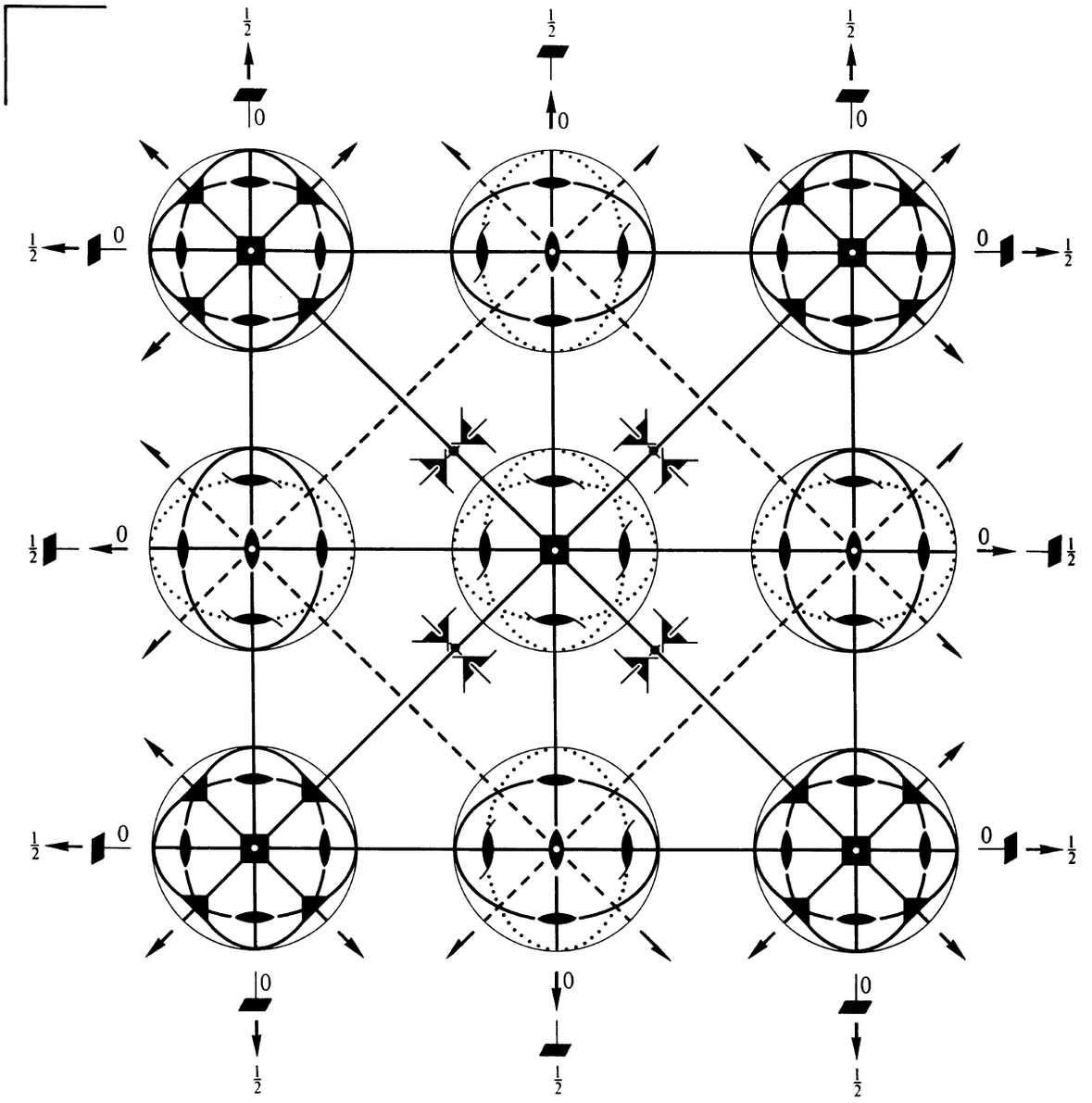
Along [001] $p4gm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,\frac{1}{4},z$

Along [111] $p31m$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c1m1$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},0$

$Pm\bar{3}m$ O_h^1 $m\bar{3}m$ Cubic

No. 221 $P\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $Pm\bar{3}m$



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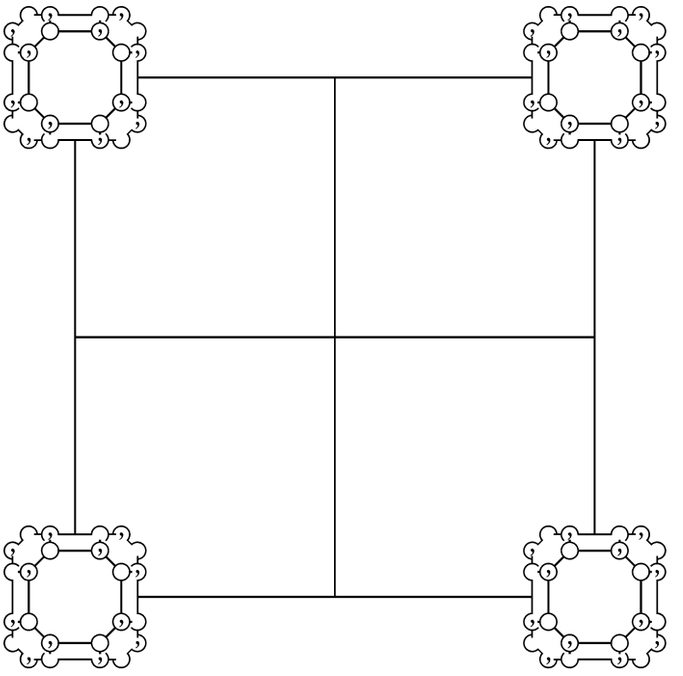


Origin at centre $(m\bar{3}m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

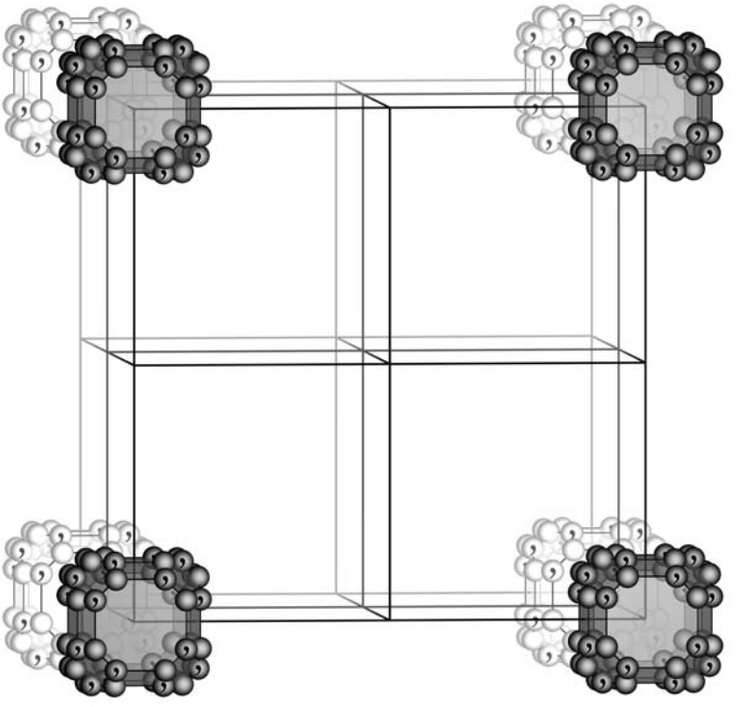
Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) 2 $0,y,0$
(4) 2 $x,0,0$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x,\bar{x}$
(7) 3^+ $x,\bar{x},\bar{x}$
(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x},\bar{x}$
(11) 3^- $\bar{x},\bar{x},x$
(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$
(14) 2 $x,\bar{x},0$
(15) 4^- $0,0,z$
(16) 4^+ $0,0,z$
(17) 4^- $x,0,0$
(18) 2 $0,y,y$
(19) 2 $0,y,\bar{y}$
(20) 4^+ $x,0,0$
(21) 4^+ $0,y,0$
(22) 2 $x,0,x$
(23) 4^- $0,y,0$
(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $0,0,0$
(26) m $x,y,0$
(27) m $x,0,z$
(28) m $0,y,z$
(29) $\bar{3}^+$ x,x,x; $0,0,0$
(30) $\bar{3}^+$ $\bar{x},x,\bar{x}$; $0,0,0$
(31) $\bar{3}^+$ $x,\bar{x},\bar{x}$; $0,0,0$
(32) $\bar{3}^+$ $\bar{x},\bar{x},x$; $0,0,0$
(33) $\bar{3}^-$ x,x,x; $0,0,0$
(34) $\bar{3}^-$ $x,\bar{x},\bar{x}$; $0,0,0$
(35) $\bar{3}^-$ $\bar{x},\bar{x},x$; $0,0,0$
(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$; $0,0,0$
(37) m $x,\bar{x},z$
(38) m x,x,z
(39) $\bar{4}^-$ $0,0,z$; $0,0,0$
(40) $\bar{4}^+$ $0,0,z$; $0,0,0$
(41) $\bar{4}^-$ $x,0,0$; $0,0,0$
(42) m $x,y,\bar{y}$
(43) m x,y,y
(44) $\bar{4}^+$ $x,0,0$; $0,0,0$
(45) $\bar{4}^+$ $0,y,0$; $0,0,0$
(46) m $\bar{x},y,x$
(47) $\bar{4}^-$ $0,y,0$; $0,0,0$
(48) m x,y,x

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		h,k,l permutable
		General:
48 n 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$ (9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$ (13) $y,x,\bar{z}$ (14) $\bar{y},\bar{x},\bar{z}$ (15) $y,\bar{x},z$ (16) $\bar{y},x,z$ (17) $x,z,\bar{y}$ (18) $\bar{x},z,y$ (19) $\bar{x},\bar{z},\bar{y}$ (20) $x,\bar{z},y$ (21) $z,y,\bar{x}$ (22) $z,\bar{y},x$ (23) $\bar{z},y,x$ (24) $\bar{z},\bar{y},\bar{x}$ (25) $\bar{x},\bar{y},\bar{z}$ (26) $x,y,\bar{z}$ (27) $x,\bar{y},z$ (28) $\bar{x},y,z$ (29) $\bar{z},\bar{x},\bar{y}$ (30) $\bar{z},x,y$ (31) $z,x,\bar{y}$ (32) $z,\bar{x},y$ (33) $\bar{y},\bar{z},\bar{x}$ (34) $y,\bar{z},x$ (35) $\bar{y},z,x$ (36) $y,z,\bar{x}$ (37) $\bar{y},\bar{x},z$ (38) y,x,z (39) $\bar{y},x,\bar{z}$ (40) $y,\bar{x},\bar{z}$ (41) $\bar{x},\bar{z},y$ (42) $x,\bar{z},\bar{y}$ (43) x,z,y (44) $\bar{x},z,\bar{y}$ (45) $\bar{z},\bar{y},x$ (46) $\bar{z},y,\bar{x}$ (47) $z,\bar{y},\bar{x}$ (48) z,y,x	no conditions
		Special: no extra conditions
24 m . . m	x,x,z $\bar{x},\bar{x},z$ $\bar{x},x,\bar{z}$ $x,\bar{x},\bar{z}$ z,x,x $z,\bar{x},\bar{x}$ $\bar{z},\bar{x},x$ $\bar{z},x,\bar{x}$ x,z,x $\bar{x},z,\bar{x}$ $x,\bar{z},\bar{x}$ $\bar{x},\bar{z},x$ $x,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{x},z$ $\bar{x},x,z$ $x,z,\bar{x}$ $\bar{x},z,x$ $\bar{x},\bar{z},\bar{x}$ $x,\bar{z},x$ $z,x,\bar{x}$ $z,\bar{x},x$ $\bar{z},x,x$ $\bar{z},\bar{x},\bar{x}$	
24 l m . .	$\frac{1}{2},y,z$ $\frac{1}{2},\bar{y},z$ $\frac{1}{2},y,\bar{z}$ $\frac{1}{2},\bar{y},\bar{z}$ $z,\frac{1}{2},y$ $z,\frac{1}{2},\bar{y}$ $\bar{z},\frac{1}{2},y$ $\bar{z},\frac{1}{2},\bar{y}$ $y,z,\frac{1}{2}$ $\bar{y},z,\frac{1}{2}$ $y,\bar{z},\frac{1}{2}$ $\bar{y},\bar{z},\frac{1}{2}$ $y,\frac{1}{2},\bar{z}$ $\bar{y},\frac{1}{2},\bar{z}$ $y,\frac{1}{2},z$ $\bar{y},\frac{1}{2},z$ $\frac{1}{2},z,\bar{y}$ $\frac{1}{2},z,y$ $\frac{1}{2},\bar{z},\bar{y}$ $\frac{1}{2},\bar{z},y$ $z,y,\frac{1}{2}$ $z,\bar{y},\frac{1}{2}$ $\bar{z},y,\frac{1}{2}$ $\bar{z},\bar{y},\frac{1}{2}$	
24 k m . .	$0,y,z$ $0,\bar{y},z$ $0,y,\bar{z}$ $0,\bar{y},\bar{z}$ $z,0,y$ $z,0,\bar{y}$ $\bar{z},0,y$ $\bar{z},0,\bar{y}$ $y,z,0$ $\bar{y},z,0$ $y,\bar{z},0$ $\bar{y},\bar{z},0$ $y,0,\bar{z}$ $\bar{y},0,\bar{z}$ $y,0,z$ $\bar{y},0,z$ $0,z,\bar{y}$ $0,z,y$ $0,\bar{z},\bar{y}$ $0,\bar{z},y$ $z,y,0$ $z,\bar{y},0$ $\bar{z},y,0$ $\bar{z},\bar{y},0$	
12 j m . $m2$	$\frac{1}{2},y,y$ $\frac{1}{2},\bar{y},y$ $\frac{1}{2},y,\bar{y}$ $\frac{1}{2},\bar{y},\bar{y}$ $y,\frac{1}{2},y$ $y,\frac{1}{2},\bar{y}$ $\bar{y},\frac{1}{2},y$ $\bar{y},\frac{1}{2},\bar{y}$ $y,y,\frac{1}{2}$ $\bar{y},y,\frac{1}{2}$ $y,\bar{y},\frac{1}{2}$ $\bar{y},\bar{y},\frac{1}{2}$	
12 i m . $m2$	$0,y,y$ $0,\bar{y},y$ $0,y,\bar{y}$ $0,\bar{y},\bar{y}$ $y,0,y$ $y,0,\bar{y}$ $\bar{y},0,y$ $\bar{y},0,\bar{y}$ $y,y,0$ $\bar{y},y,0$ $y,\bar{y},0$ $\bar{y},\bar{y},0$	
12 h m m 2 . .	$x,\frac{1}{2},0$ $\bar{x},\frac{1}{2},0$ $0,x,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $\frac{1}{2},0,x$ $\frac{1}{2},0,\bar{x}$ $\frac{1}{2},x,0$ $\frac{1}{2},\bar{x},0$ $x,0,\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$ $0,\frac{1}{2},\bar{x}$ $0,\frac{1}{2},x$	
8 g . 3 m	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x,x,\bar{x}$ $\bar{x},\bar{x},\bar{x}$ $x,\bar{x},x$ $\bar{x},x,x$	
6 f 4 m . m	$x,\frac{1}{2},\frac{1}{2}$ $\bar{x},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},x,\frac{1}{2}$ $\frac{1}{2},\bar{x},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},x$ $\frac{1}{2},\frac{1}{2},\bar{x}$	
6 e 4 m . m	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$	
3 d $4/m$ m . m	$\frac{1}{2},0,0$ $0,\frac{1}{2},0$ $0,0,\frac{1}{2}$	
3 c $4/m$ m . m	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$	
1 b $m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
1 a $m\bar{3}m$	$0,0,0$	



Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

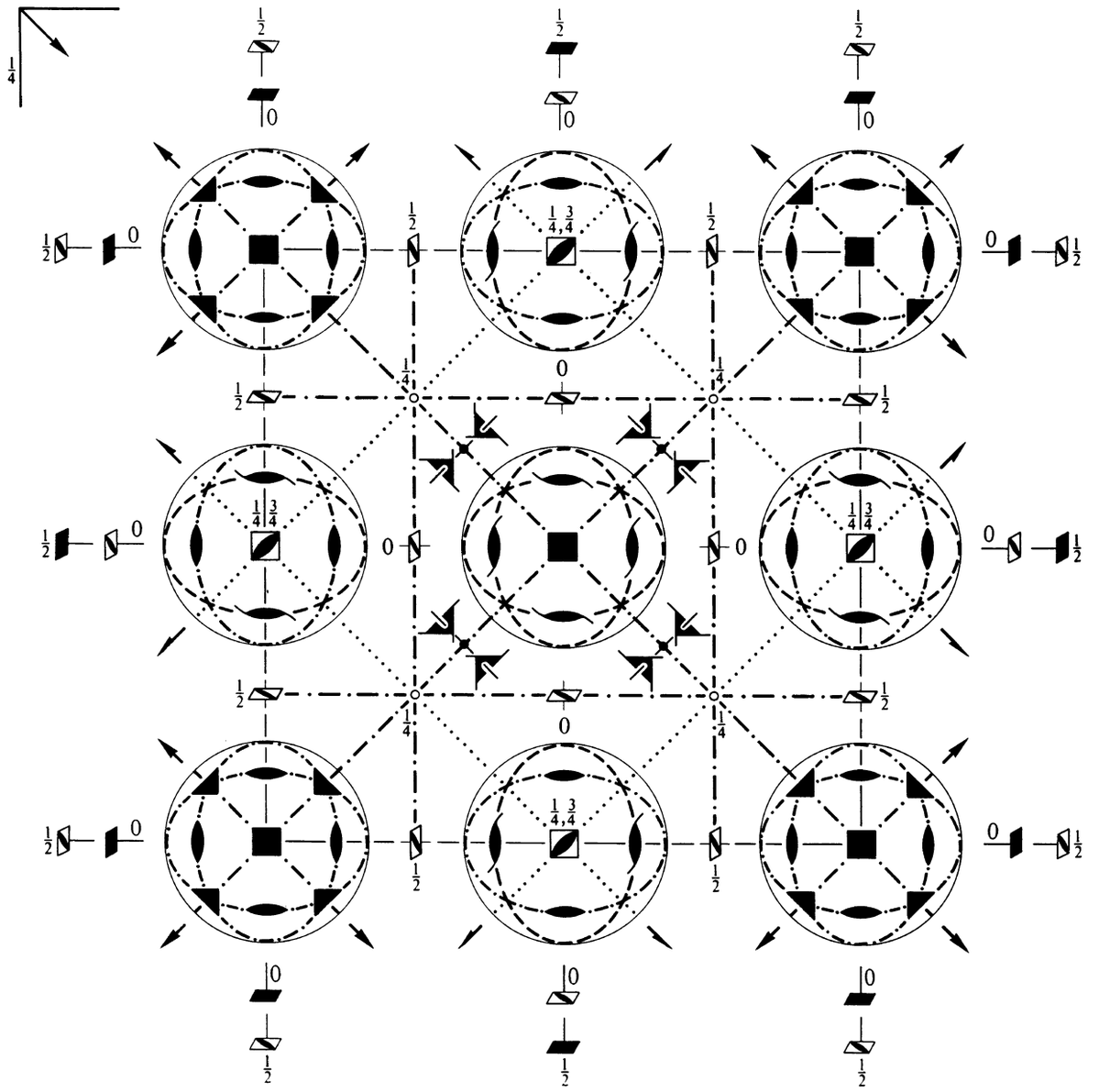
Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$Pn\bar{3}n$ O_h^2 $m\bar{3}m$ Cubic

No. 222 $P\ 4/n\ \bar{3}\ 2/n$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 1



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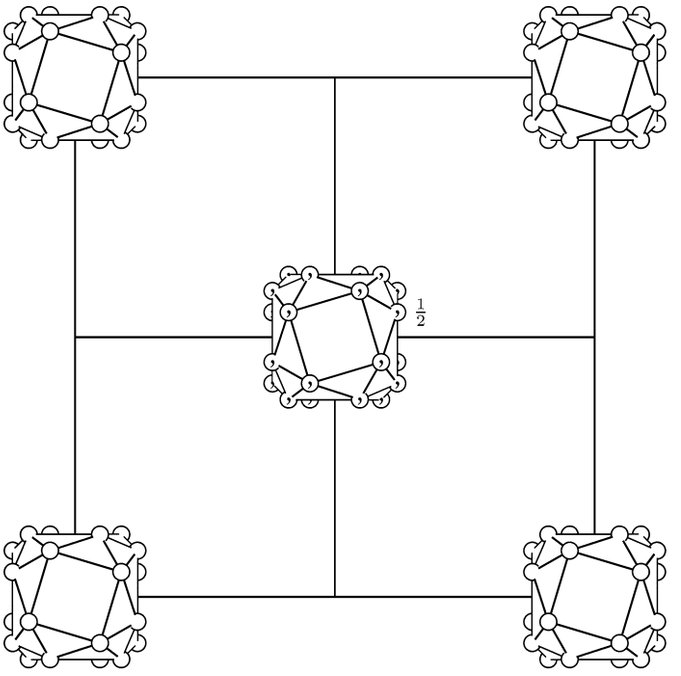


Origin at 4 3 2, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre $(\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Symmetry operations

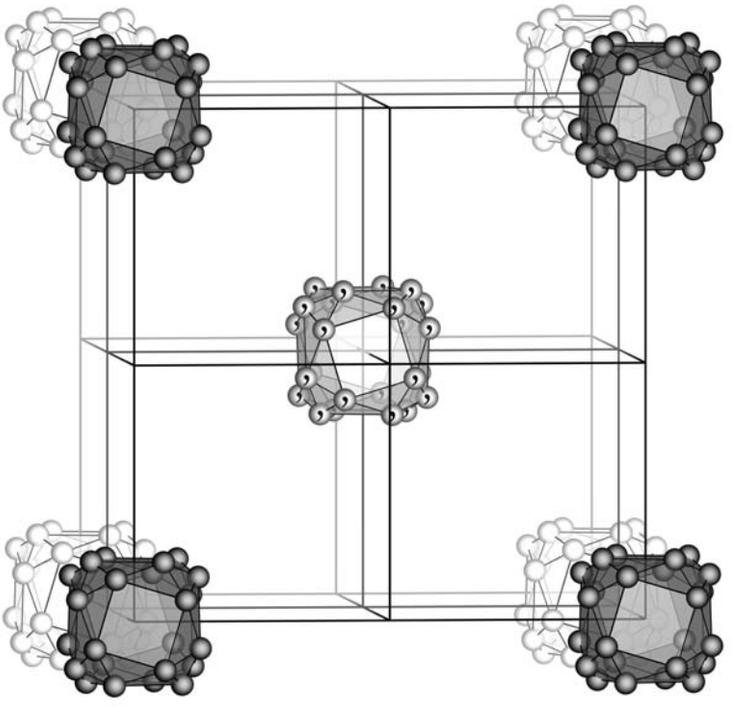
(1) 1
(2) 2 $0,0,z$
(3) 2 $0,y,0$
(4) 2 $x,0,0$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x,\bar{x}$
(7) 3^+ $x,\bar{x},\bar{x}$
(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x},\bar{x}$
(11) 3^- $\bar{x},\bar{x},x$
(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 $x,x,0$
(14) 2 $x,\bar{x},0$
(15) 4^- $0,0,z$
(16) 4^+ $0,0,z$
(17) 4^- $x,0,0$
(18) 2 $0,y,y$
(19) 2 $0,y,\bar{y}$
(20) 4^+ $x,0,0$
(21) 4^+ $0,y,0$
(22) 2 $x,0,x$
(23) 4^- $0,y,0$
(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(26) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$
(27) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$
(28) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(29) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(30) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{1}{4},\frac{1}{4},\frac{3}{4}$
(31) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}$; $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$
(32) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(33) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$
(35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$
(36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$
(37) c $x+\frac{1}{2},\bar{x},z$
(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z
(39) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^-$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$
(42) a $x,y+\frac{1}{2},\bar{y}$
(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$
(46) b $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$
(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

ORIGIN CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable
							General:
48	i	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	$0kl$: $k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	hhl: $l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	$h00$: $h=2n$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$	
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$	
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$	
			(25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	
			(29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	
							Special: as above, plus
24	h	. . 2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	hkl: $h+k+l=2n$
			$y,0,y$	$y,0,\bar{y}$	$\bar{y},0,y$	$\bar{y},0,\bar{y}$	
			$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$	
			$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},y+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},y+\frac{1}{2}$	
			$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},y+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},\bar{y}+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},y+\frac{1}{2}$	
			$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	
24	g	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	hkl: $h+k+l=2n$
			$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},0,\bar{x}$	$\frac{1}{2},0,x$	
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\bar{x}+\frac{1}{2}$	$\frac{1}{2},0,x+\frac{1}{2}$	
			$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},0$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$x+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},x+\frac{1}{2}$	$0,\frac{1}{2},\bar{x}+\frac{1}{2}$	
16	f	. 3 .	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$	hkl: $h+k+l=2n$
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$	
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	
12	e	4 . .	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	hkl: $h+k+l=2n$
			$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	
12	d	$\bar{4}$ . .	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl: $h+k+l=2n$
			$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	
8	c	. $\bar{3}$.	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h,k,l=2n$
6	b	4 2 . 2	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$	hkl: $h+k+l=2n$
2	a	4 3 2	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$



Symmetry of special projections

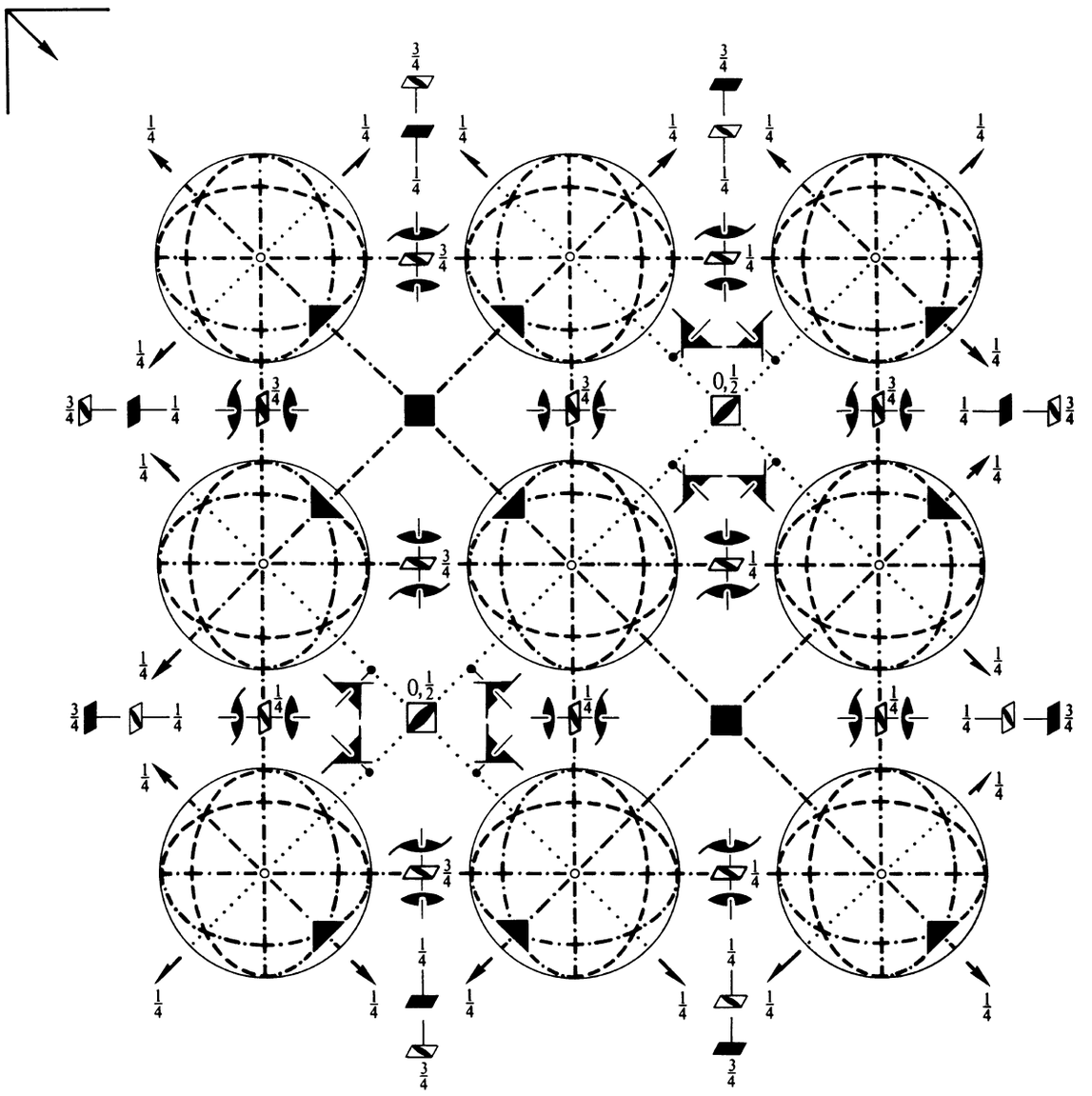
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

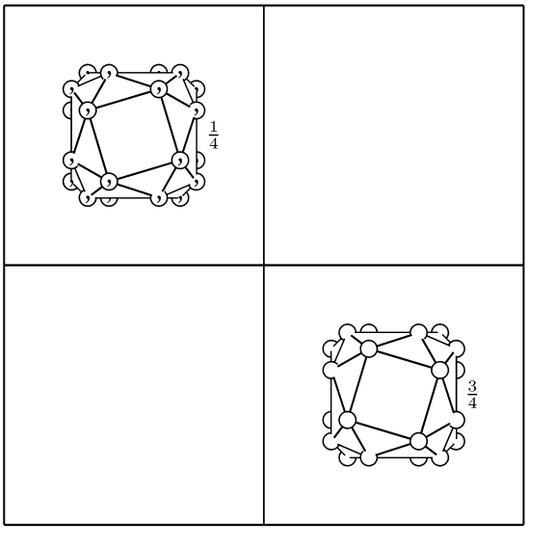
Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

No. 222 $P\ 4/n\ \bar{3}\ 2/n$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 2





Origin at centre $(\bar{3})$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from 4 3 2

Asymmetric unit $\frac{1}{4} \le x \le \frac{3}{4}$; $\frac{1}{4} \le y \le \frac{3}{4}$; $\frac{1}{4} \le z \le \frac{3}{4}$; $y \le x$; $z \le y$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$

Symmetry operations

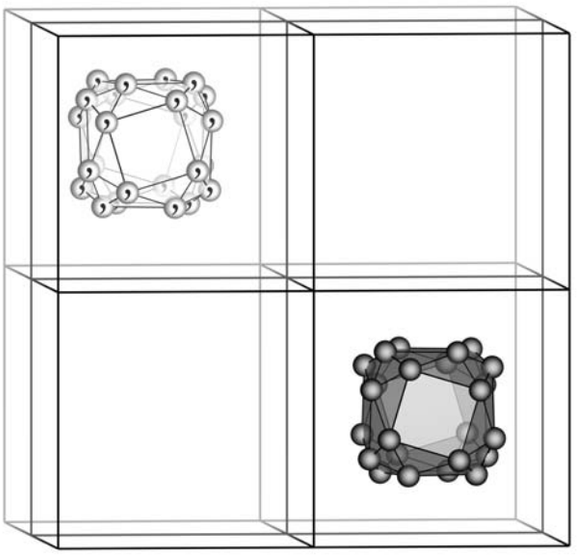
(1) 1
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) 2 $\frac{1}{4},y,\frac{1}{4}$
(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x
(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) 2 $x,x,\frac{1}{4}$
(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(15) 4^- $\frac{1}{4},\frac{1}{4},z$
(16) 4^+ $\frac{1}{4},\frac{1}{4},z$
(17) 4^- $x,\frac{1}{4},\frac{1}{4}$
(18) 2 $\frac{1}{4},y,y$
(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$
(20) 4^+ $x,\frac{1}{4},\frac{1}{4}$
(21) 4^+ $\frac{1}{4},y,\frac{1}{4}$
(22) 2 $x,\frac{1}{4},x$
(23) 4^- $\frac{1}{4},y,\frac{1}{4}$
(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}$ 0,0,0
(26) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(27) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$
(28) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
(29) $\bar{3}^+$ x,x,x; 0,0,0
(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; $-\frac{1}{2},0,\frac{1}{2}$
(31) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+1,\bar{x}$; $0,\frac{1}{2},-\frac{1}{2}$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{1}{2},-\frac{1}{2},0$
(33) $\bar{3}^-$ x,x,x; 0,0,0
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-1,\bar{x}$; $0,-\frac{1}{2},\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; $-\frac{1}{2},\frac{1}{2},0$
(36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,-\frac{1}{2}$
(37) c $x,\bar{x},z$
(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z
(39) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$
(40) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$
(41) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}$; $0,-\frac{1}{4},\frac{1}{4}$
(42) a $x,y,\bar{y}$
(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}$; $0,\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},0,\frac{1}{4}$
(46) b $\bar{x},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},0,-\frac{1}{4}$
(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

ORIGIN CHOICE 2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates								Reflection conditions
											h,k,l permutable General:
48	i	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$					$0kl$: $k+l=2n$ hhl: $l=2n$ $h00$: $h=2n$
			(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$					
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$					
			(13) $y,x,\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y,\bar{x}+\frac{1}{2},z$	(16) $\bar{y}+\frac{1}{2},x,z$					
			(17) $x,z,\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z,y$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x,\bar{z}+\frac{1}{2},y$					
			(21) $z,y,\bar{x}+\frac{1}{2}$	(22) $z,\bar{y}+\frac{1}{2},x$	(23) $\bar{z}+\frac{1}{2},y,x$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$					
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(27) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(28) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$					
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(32) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$					
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(35) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$					
			(37) $\bar{y},\bar{x},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y},x+\frac{1}{2},\bar{z}$	(40) $y+\frac{1}{2},\bar{x},\bar{z}$					
			(41) $\bar{x},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z},\bar{y}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x},z+\frac{1}{2},\bar{y}$					
			(45) $\bar{z},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}$	(47) $z+\frac{1}{2},\bar{y},\bar{x}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$					
											Special: as above, plus
24	h	. . 2	$\frac{1}{4},y,y$	$\frac{1}{4},\bar{y}+\frac{1}{2},y$	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{1}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2}$					hkl: $h+k+l=2n$
			$y,\frac{1}{4},y$	$y,\frac{1}{4},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}+\frac{1}{2}$					
			$y,y,\frac{1}{4}$	$\bar{y}+\frac{1}{2},y,\frac{1}{4}$	$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{4}$					
			$\frac{3}{4},\bar{y},\bar{y}$	$\frac{3}{4},y+\frac{1}{2},\bar{y}$	$\frac{3}{4},\bar{y},y+\frac{1}{2}$	$\frac{3}{4},y+\frac{1}{2},y+\frac{1}{2}$					
			$\bar{y},\frac{3}{4},\bar{y}$	$\bar{y},\frac{3}{4},y+\frac{1}{2}$	$y+\frac{1}{2},\frac{3}{4},\bar{y}$	$y+\frac{1}{2},\frac{3}{4},y+\frac{1}{2}$					
			$\bar{y},\bar{y},\frac{3}{4}$	$y+\frac{1}{2},\bar{y},\frac{3}{4}$	$\bar{y},y+\frac{1}{2},\frac{3}{4}$	$y+\frac{1}{2},y+\frac{1}{2},\frac{3}{4}$					
24	g	2 . .	$x,\frac{3}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$			hkl: $h+k+l=2n$
			$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}+\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},x$			
			$\bar{x},\frac{1}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{1}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x+\frac{1}{2}$			
			$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x+\frac{1}{2},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},x+\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},\bar{x}$			
16	f	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$					hkl: $h+k+l=2n$
			$x,x,\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,x$					
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},x+\frac{1}{2}$					
			$\bar{x},\bar{x},x+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}$					
12	e	4 . .	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$			hkl: $h+k+l=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$			
12	d	$\bar{4}$ . .	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $h+k+l=2n$
			$\frac{3}{4},0,\frac{1}{4}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$			
8	c	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	hkl: $h,k,l=2n$
6	b	4 2 . 2	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$			hkl: $h+k+l=2n$
2	a	4 3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$							hkl: $h+k+l=2n$



Symmetry of special projections

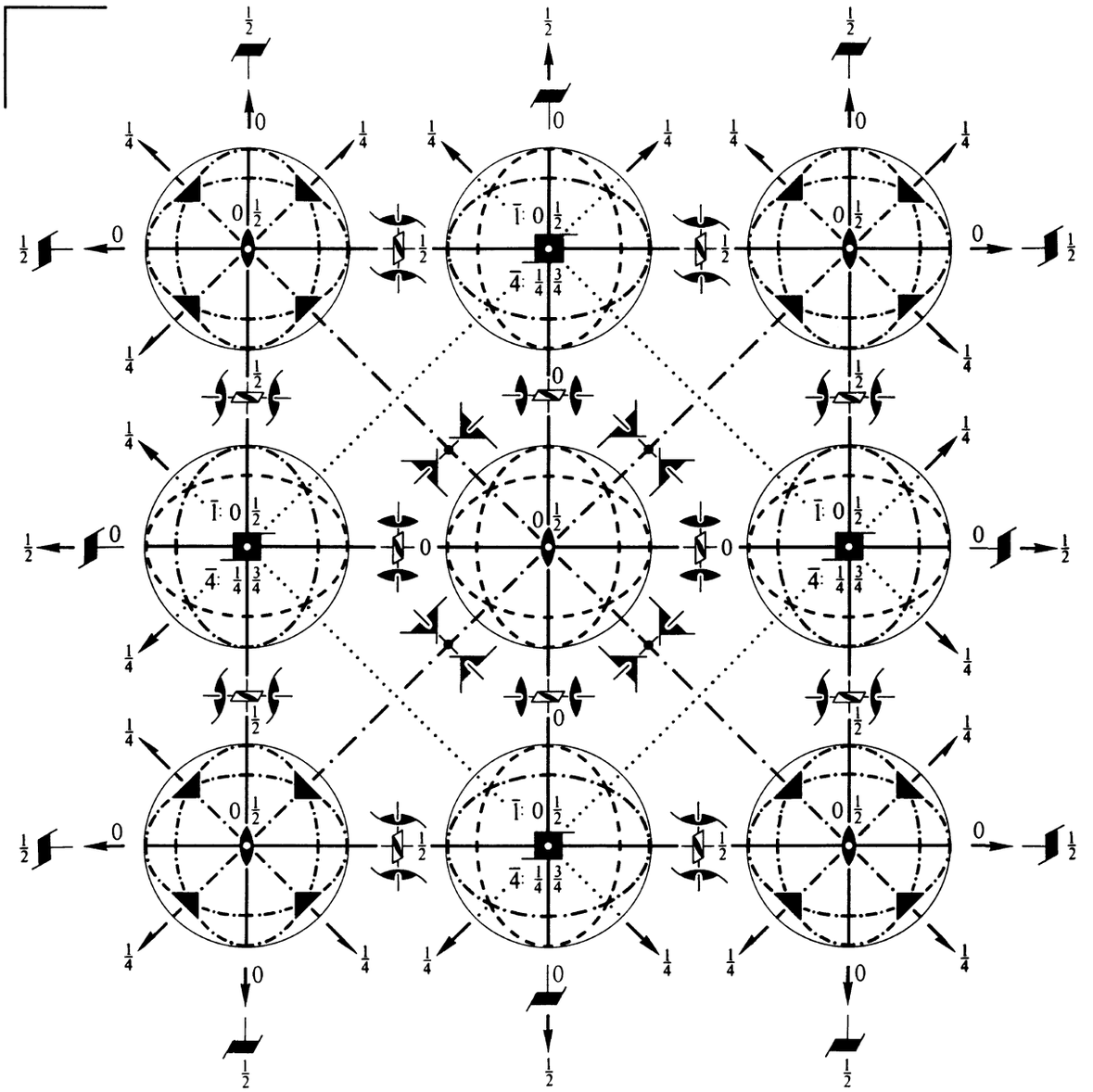
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$Pm\bar{3}n$ O_h^3 $m\bar{3}m$ Cubic

No. 223 $P\ 4_2/m\ \bar{3}\ 2/n$ Patterson symmetry $Pm\bar{3}m$



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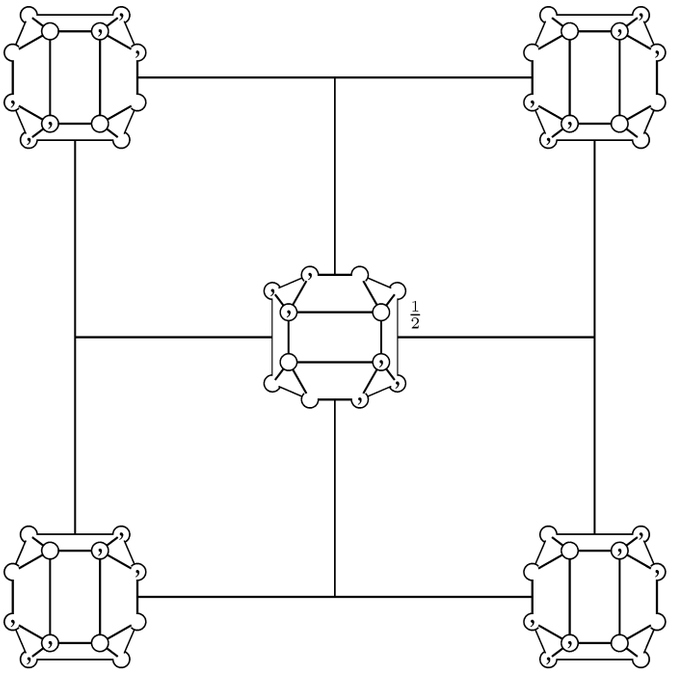


Origin at centre $(m\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{4}; \quad z \le \min(x, \frac{1}{2}-x, y, \frac{1}{2}-y)$

Vertices $0,0,0 \quad \frac{1}{2},0,0 \quad \frac{1}{2},\frac{1}{2},0 \quad 0,\frac{1}{2},0 \quad \frac{1}{4},\frac{1}{4},\frac{1}{4}$

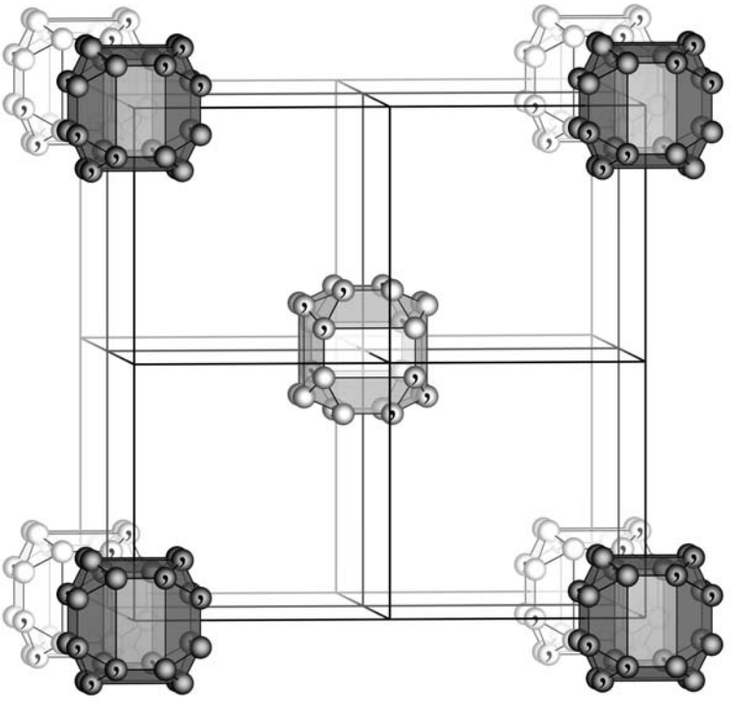
Symmetry operations

(1) 1
(2) 2 $0,0,z$
(3) 2 $0,y,0$
(4) 2 $x,0,0$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x,\bar{x}$
(7) 3^+ $x,\bar{x},\bar{x}$
(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x},\bar{x}$
(11) 3^- $\bar{x},\bar{x},x$
(12) 3^- $\bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$
(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(16) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{2},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,y$
(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$
(20) $4^+(\frac{1}{2},0,0)$ $x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{2},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},x$
(23) $4^-(0,\frac{1}{2},0)$ $0,y,\frac{1}{2}$
(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}$ $0,0,0$
(26) m $x,y,0$
(27) m $x,0,z$
(28) m $0,y,z$
(29) $\bar{3}^+$ $x,x,x;\ 0,0,0$
(30) $\bar{3}^+$ $\bar{x},x,\bar{x};\ 0,0,0$
(31) $\bar{3}^+$ $x,\bar{x},\bar{x};\ 0,0,0$
(32) $\bar{3}^+$ $\bar{x},\bar{x},x;\ 0,0,0$
(33) $\bar{3}^-$ $x,x,x;\ 0,0,0$
(34) $\bar{3}^-$ $x,\bar{x},\bar{x};\ 0,0,0$
(35) $\bar{3}^-$ $\bar{x},\bar{x},x;\ 0,0,0$
(36) $\bar{3}^-$ $\bar{x},x,\bar{x};\ 0,0,0$
(37) c $x+\frac{1}{2},\bar{x},z$
(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z
(39) $\bar{4}^-$ $0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^-$ $x,0,\frac{1}{2};\ \frac{1}{4},0,\frac{1}{2}$
(42) a $x,y+\frac{1}{2},\bar{y}$
(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{2},0;\ \frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^+$ $0,y,\frac{1}{2};\ 0,\frac{1}{4},\frac{1}{2}$
(46) b $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{1}{2},y,0;\ \frac{1}{2},\frac{1}{4},0$
(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		h,k,l permutable
		General:
48 l 1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$ (5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$ (9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$ (13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ (18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ (19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$ (21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ (22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$ (23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$ (24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$ (25) $\bar{x},\bar{y},\bar{z}$ (26) $x,y,\bar{z}$ (27) $x,\bar{y},z$ (28) $\bar{x},y,z$ (29) $\bar{z},\bar{x},\bar{y}$ (30) $\bar{z},x,y$ (31) $z,x,\bar{y}$ (32) $z,\bar{x},y$ (33) $\bar{y},\bar{z},\bar{x}$ (34) $y,\bar{z},x$ (35) $\bar{y},z,x$ (36) $y,z,\bar{x}$ (37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$ (42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ (43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ (44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ (45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$ (46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$ (47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$ (48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	hhl: $l=2n$ $h00$: $h=2n$
		Special: as above, plus
24 k m . .	$0,y,z$ $0,\bar{y},z$ $0,y,\bar{z}$ $0,\bar{y},\bar{z}$ $z,0,y$ $z,0,\bar{y}$ $\bar{z},0,y$ $\bar{z},0,\bar{y}$ $y,z,0$ $\bar{y},z,0$ $y,\bar{z},0$ $\bar{y},\bar{z},0$ $y+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$ $\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$ $\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$ $\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$ $z+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$ $z+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$ $\bar{z}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$ $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	no extra conditions
24 j . . 2	$\frac{1}{4},y,y+\frac{1}{2}$ $\frac{3}{4},\bar{y},y+\frac{1}{2}$ $\frac{3}{4},y,\bar{y}+\frac{1}{2}$ $\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},y$ $y+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y}+\frac{1}{2},\frac{3}{4},y$ $\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$ $y,y+\frac{1}{2},\frac{1}{4}$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$ $y,\bar{y}+\frac{1}{2},\frac{3}{4}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\frac{1}{4},\bar{y},y+\frac{1}{2}$ $\frac{3}{4},y,y+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $y+\frac{1}{2},\frac{3}{4},y$ $\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$ $y,y+\frac{1}{2},\frac{3}{4}$	hkl: $h=2n$
16 i . 3 .	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ $\bar{x},\bar{x},\bar{x}$ $x,x,\bar{x}$ $x,\bar{x},x$ $\bar{x},x,x$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$ $x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	hkl: $h+k+l=2n$
12 h $m\,m$ 2 . .	$x,\frac{1}{2},0$ $\bar{x},\frac{1}{2},0$ $0,x,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$ $\frac{1}{2},0,x$ $\frac{1}{2},0,\bar{x}$ $0,x+\frac{1}{2},\frac{1}{2}$ $0,\bar{x}+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},0$ $\bar{x}+\frac{1}{2},\frac{1}{2},0$ $\frac{1}{2},0,\bar{x}+\frac{1}{2}$ $\frac{1}{2},0,x+\frac{1}{2}$	hkl: $h=2n$
12 g $m\,m$ 2 . .	$x,0,\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$ $\frac{1}{2},x,0$ $\frac{1}{2},\bar{x},0$ $0,\frac{1}{2},x$ $0,\frac{1}{2},\bar{x}$ $\frac{1}{2},x+\frac{1}{2},0$ $\frac{1}{2},\bar{x}+\frac{1}{2},0$ $x+\frac{1}{2},0,\frac{1}{2}$ $\bar{x}+\frac{1}{2},0,\frac{1}{2}$ $0,\frac{1}{2},\bar{x}+\frac{1}{2}$ $0,\frac{1}{2},x+\frac{1}{2}$	hkl: $h=2n$
12 f $m\,m$ 2 . .	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$ $\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	hkl: $h+k+l=2n$
8 e . 3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{1}{4}$ $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ $\frac{3}{4},\frac{3}{4},\frac{3}{4}$ $\frac{1}{4},\frac{1}{4},\frac{3}{4}$ $\frac{1}{4},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h,k,l=2n$
6 d $\bar{4}\,m$. 2	$\frac{1}{4},\frac{1}{2},0$ $\frac{3}{4},\frac{1}{2},0$ $0,\frac{1}{4},\frac{1}{2}$ $0,\frac{3}{4},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{1}{2},0,\frac{3}{4}$	hkl: $h+k+l=2n$ or $h=2n+1$, $k=4n$ and $l=4n+2$
6 c $\bar{4}\,m$. 2	$\frac{1}{4},0,\frac{1}{2}$ $\frac{3}{4},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{4},0$ $\frac{1}{2},\frac{3}{4},0$ $0,\frac{1}{2},\frac{1}{4}$ $0,\frac{1}{2},\frac{3}{4}$	
6 b $m\,m\,m$ . .	$0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$ $0,\frac{1}{2},0$ $\frac{1}{2},0,0$ $0,0,\frac{1}{2}$	hkl: $h+k+l=2n$
2 a $m\bar{3}$.	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$



Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0, \frac{1}{2}, z$

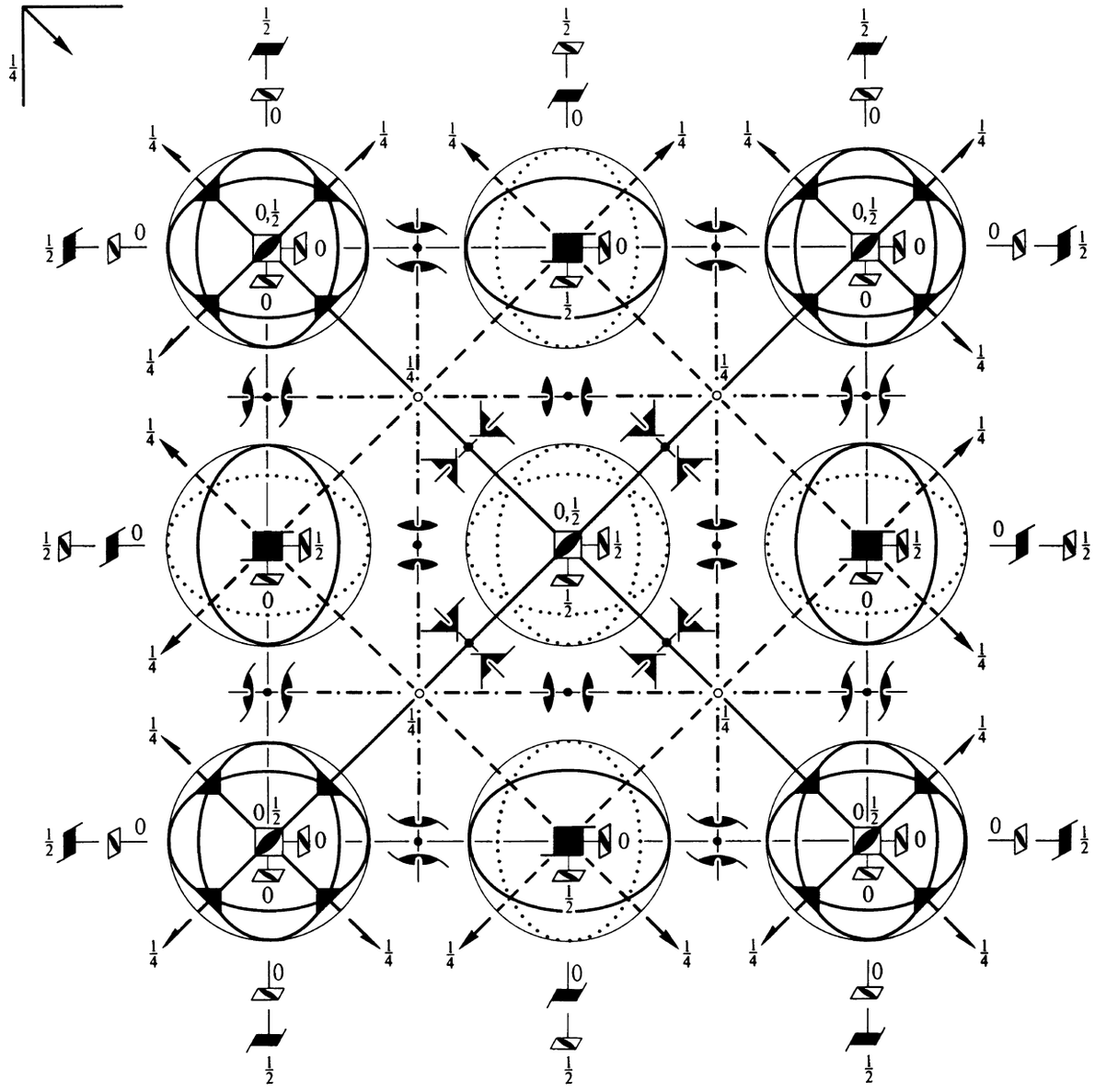
Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a} - \mathbf{b} - \mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a} + 2\mathbf{b} - \mathbf{c})$
Origin at x, x, x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a} + \mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x, x, 0$

$Pn\bar{3}m$ O_h^4 $m\bar{3}m$ Cubic

No. 224 $P4_2/n\bar{3}2/m$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 1



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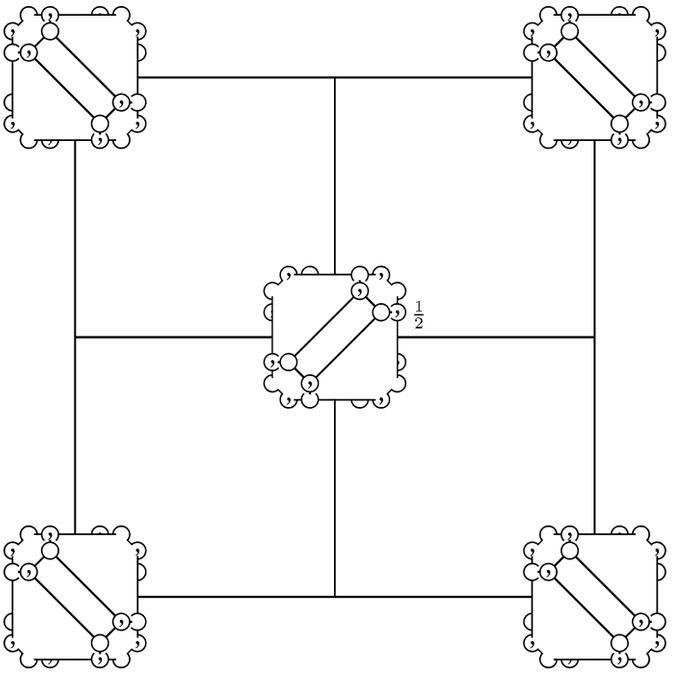


Origin at $\bar{4}\,3\,m$, at $-\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$ from centre $(\bar{3}\,m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $-\frac{1}{4} \le z \le \frac{1}{4}$; $y \le x$; $\max(x-\frac{1}{2},-y) \le z \le \min(\frac{1}{2}-x,y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$

Symmetry operations

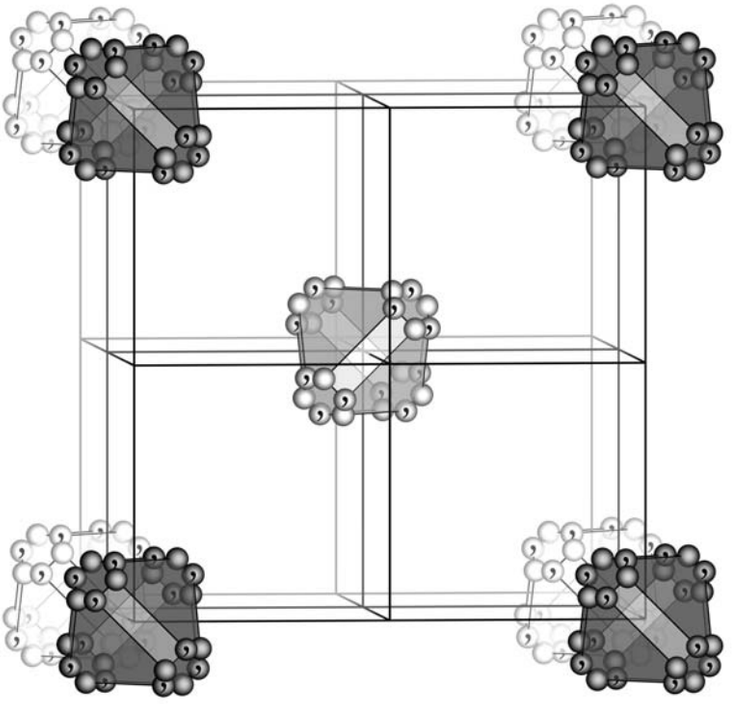
(1) 1
(2) 2 0,0,z
(3) 2 0,y,0
(4) 2 x,0,0
(5) 3^+ x,x,x
(6) 3^+ $\bar{x}$,x,$\bar{x}$
(7) 3^+ x,$\bar{x}$,$\bar{x}$
(8) 3^+ $\bar{x}$,$\bar{x}$,x
(9) 3^- x,x,x
(10) 3^- x,$\bar{x}$,$\bar{x}$
(11) 3^- $\bar{x}$,$\bar{x}$,x
(12) 3^- $\bar{x}$,x,$\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ x,x,$\frac{1}{4}$
(14) 2 x,$\bar{x}+\frac{1}{2}$,$\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2}$,0,z
(16) $4^+(0,0,\frac{1}{2})$ 0,$\frac{1}{2}$,z
(17) $4^-(\frac{1}{2},0,0)$ x,$\frac{1}{2}$,0
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4}$,y,y
(19) 2 $\frac{1}{4}$,$y+\frac{1}{2}$,$\bar{y}$
(20) $4^+(\frac{1}{2},0,0)$ x,0,$\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{2}$,y,0
(22) $2(\frac{1}{2},0,\frac{1}{2})$ x,$\frac{1}{4}$,x
(23) $4^-(0,\frac{1}{2},0)$ 0,y,$\frac{1}{2}$
(24) 2 $\bar{x}+\frac{1}{2}$,$\frac{1}{4}$,x
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(26) $n(\frac{1}{2},\frac{1}{2},0)$ x,y,$\frac{1}{4}$
(27) $n(\frac{1}{2},0,\frac{1}{2})$ x,$\frac{1}{4}$,z
(28) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4}$,y,z
(29) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(30) $\bar{3}^+$ $\bar{x}-1$,$x+1$,$\bar{x}$; $-\frac{1}{4},\frac{1}{4},\frac{3}{4}$
(31) $\bar{3}^+$ x,$\bar{x}+1$,$\bar{x}$; $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$
(32) $\bar{3}^+$ $\bar{x}+1$,$\bar{x}$,x; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(33) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(34) $\bar{3}^-$ $x+1$,$\bar{x}-1$,$\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$
(35) $\bar{3}^-$ $\bar{x}$,$\bar{x}+1$,x; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$
(36) $\bar{3}^-$ $\bar{x}+1$,x,$\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$
(37) m x,$\bar{x}$,z
(38) m x,x,z
(39) $\bar{4}^-$ 0,0,z; 0,0,0
(40) $\bar{4}^+$ 0,0,z; 0,0,0
(41) $\bar{4}^-$ x,0,0; 0,0,0
(42) m x,y,$\bar{y}$
(43) m x,y,y
(44) $\bar{4}^+$ x,0,0; 0,0,0
(45) $\bar{4}^+$ 0,y,0; 0,0,0
(46) m $\bar{x}$,y,x
(47) $\bar{4}^-$ 0,y,0; 0,0,0
(48) m x,y,x

ORIGIN CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable General:
48	l	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	$0kl$: $k+l=2n$ $h00$: $h=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			(25) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	
			(29) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{2},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(33) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(34) $y+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$	
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$	
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x	
							Special: as above, plus
24	k	. . m	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	no extra conditions
			z,x,x	$z,\bar{x},\bar{x}$	$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	
			x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$	
			$x+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	
			$x+\frac{1}{2},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},z+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	
			$z+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$z+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{z}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	
24	j	. . 2	$\frac{1}{4},y,y+\frac{1}{2}$	$\frac{3}{4},\bar{y},y+\frac{1}{2}$	$\frac{3}{4},y,\bar{y}+\frac{1}{2}$	$\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{4},y$	$y+\frac{1}{2},\frac{3}{4},\bar{y}$	no extra conditions
			$\bar{y}+\frac{1}{2},\frac{3}{4},y$	$\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$	$y,y+\frac{1}{2},\frac{1}{4}$	$\bar{y},y+\frac{1}{2},\frac{3}{4}$	$y,\bar{y}+\frac{1}{2},\frac{3}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$	
			$\frac{1}{4},\bar{y}+\frac{1}{2},\bar{y}$	$\frac{3}{4},y+\frac{1}{2},\bar{y}$	$\frac{3}{4},\bar{y}+\frac{1}{2},y$	$\frac{1}{4},y+\frac{1}{2},y$	$\bar{y},\frac{1}{4},\bar{y}+\frac{1}{2}$	$\bar{y},\frac{3}{4},y+\frac{1}{2}$	
			$y,\frac{3}{4},\bar{y}+\frac{1}{2}$	$y,\frac{1}{4},y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{y},\frac{1}{4}$	$y+\frac{1}{2},\bar{y},\frac{3}{4}$	$\bar{y}+\frac{1}{2},y,\frac{3}{4}$	$y+\frac{1}{2},y,\frac{1}{4}$	
24	i	. . 2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{3}{4},y,y+\frac{1}{2}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$	no extra conditions
			$y+\frac{1}{2},\frac{3}{4},y$	$y+\frac{1}{2},\frac{1}{4},\bar{y}$	$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y,y+\frac{1}{2},\frac{3}{4}$	$\bar{y},y+\frac{1}{2},\frac{1}{4}$	
			$\frac{1}{4},\bar{y}+\frac{1}{2},y$	$\frac{3}{4},y+\frac{1}{2},y$	$\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}$	$\frac{1}{4},y+\frac{1}{2},\bar{y}$	$y,\frac{1}{4},\bar{y}+\frac{1}{2}$	$y,\frac{3}{4},y+\frac{1}{2}$	
			$\bar{y},\frac{3}{4},\bar{y}+\frac{1}{2}$	$\bar{y},\frac{1}{4},y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},y,\frac{1}{4}$	$y+\frac{1}{2},\bar{y},\frac{3}{4}$	$\bar{y}+\frac{1}{2},\bar{y},\frac{3}{4}$	$y+\frac{1}{2},\bar{y},\frac{1}{4}$	
24	h	2 . .	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$	hkl: $h+k+l=2n$
			$\frac{1}{2},x+\frac{1}{2},0$	$\frac{1}{2},\bar{x}+\frac{1}{2},0$	$x+\frac{1}{2},0,\frac{1}{2}$	$\bar{x}+\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}+\frac{1}{2}$	$0,\frac{1}{2},x+\frac{1}{2}$	
			$\bar{x}+\frac{1}{2},\frac{1}{2},0$	$x+\frac{1}{2},\frac{1}{2},0$	$0,\bar{x}+\frac{1}{2},\frac{1}{2}$	$0,x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\bar{x}+\frac{1}{2}$	$\frac{1}{2},0,x+\frac{1}{2}$	
			$0,\bar{x},\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\frac{1}{2},0$	$x,\frac{1}{2},0$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$	
12	g	2 . mm	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	hkl: $h+k+l=2n$
			$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$	
12	f	2 . 2 2	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	hkl: $h+k+l=2n$
			$\frac{1}{4},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{2},0$	$0,\frac{1}{4},\frac{1}{2}$	$0,\frac{3}{4},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$	
8	e	. 3 m	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$	no extra conditions
			$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	
6	d	$\bar{4}$ 2 . m	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl: $h+k+l=2n$
4	c	. $\bar{3}$ m	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	hkl: $h+k,h+l,k+l=2n$
4	b	. $\bar{3}$ m	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	hkl: $h+k,h+l,k+l=2n$
2	a	$\bar{4}$ 3 m	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+k+l=2n$



Symmetry of special projections

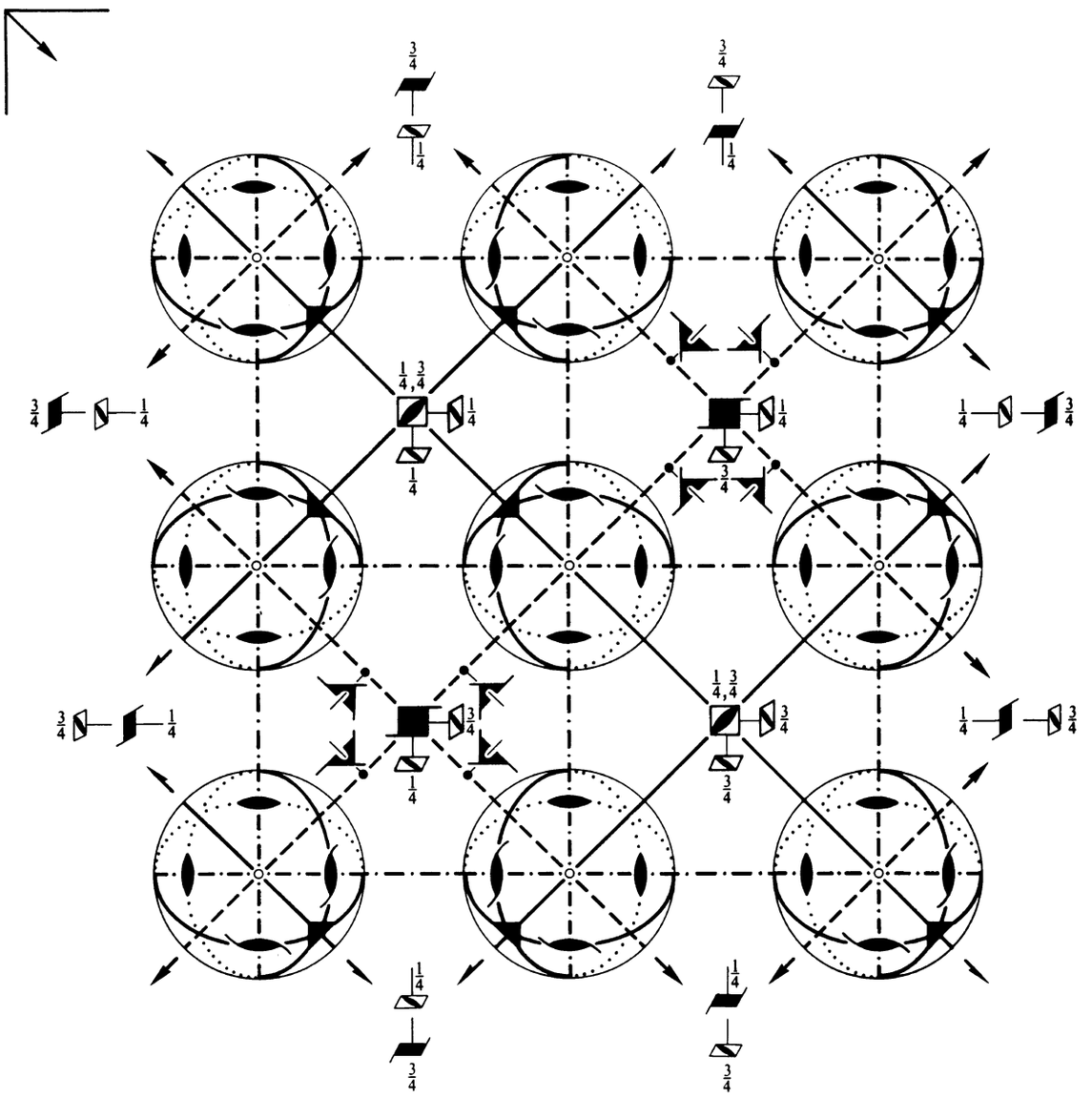
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

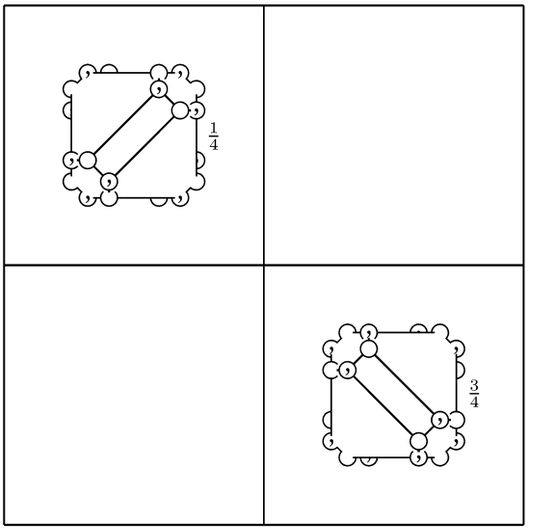
Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{4}$

No. 224 $P\ 4_2/n\ \bar{3}\ 2/m$ Patterson symmetry $Pm\bar{3}m$

ORIGIN CHOICE 2





Origin at centre $(\bar{3}m)$, at $\frac{1}{4},\frac{1}{4},\frac{1}{4}$ from $\bar{4}3m$

Asymmetric unit $\frac{1}{4}\le x\le\frac{3}{4};\quad \frac{1}{4}\le y\le\frac{3}{4};\quad 0\le z\le\frac{1}{2};\quad y\le x;\quad \max(x-\frac{1}{2},\frac{1}{2}-y)\le z\le\min(y,1-x)$

Vertices $\frac{1}{4},\frac{1}{4},\frac{1}{4}\quad \frac{3}{4},\frac{1}{4},\frac{1}{4}\quad \frac{3}{4},\frac{3}{4},\frac{1}{4}\quad \frac{1}{2},\frac{1}{2},\frac{1}{2}\quad \frac{1}{2},\frac{1}{2},0$

Symmetry operations

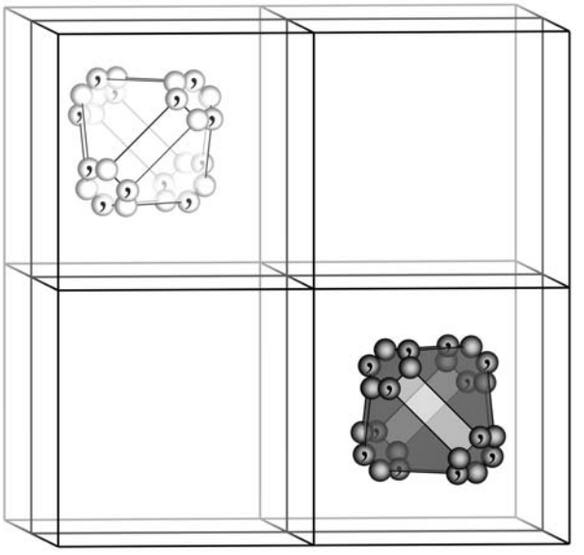
(1) 1
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) 2 $\frac{1}{4},y,\frac{1}{4}$
(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x
(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,0$
(14) 2 $x,\bar{x},0$
(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},-\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{2})$ $-\frac{1}{4},\frac{1}{4},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{4},-\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $0,y,y$
(19) 2 $0,y,\bar{y}$
(20) $4^+(\frac{1}{2},0,0)$ $x,-\frac{1}{4},\frac{1}{4}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{4},y,-\frac{1}{4}$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,0,x$
(23) $4^-(0,\frac{1}{2},0)$ $-\frac{1}{4},y,\frac{1}{4}$
(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $0,0,0$
(26) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(27) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$
(28) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
(29) $\bar{3}^+$ $x,x,x;\ 0,0,0$
(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x};\ -\frac{1}{2},0,\frac{1}{2}$
(31) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+1,\bar{x};\ 0,\frac{1}{2},-\frac{1}{2}$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x;\ \frac{1}{2},-\frac{1}{2},0$
(33) $\bar{3}^-$ $x,x,x;\ 0,0,0$
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-1,\bar{x};\ 0,-\frac{1}{2},\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x;\ -\frac{1}{2},\frac{1}{2},0$
(36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x};\ \frac{1}{2},0,-\frac{1}{2}$
(37) m $x+\frac{1}{2},\bar{x},z$
(38) m x,x,z
(39) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(42) m $x,y+\frac{1}{2},\bar{y}$
(43) m x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(46) m $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(48) m x,y,x

ORIGIN CHOICE 2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							h,k,l permutable General:
48	l	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(3) $\bar{x}+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$ $h00$: $h=2n$
			(5) z,x,y	(6) $z,\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},y$	(8) $\bar{z}+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	(11) $y,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2},x$	
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{2},\bar{x},z+\frac{1}{2}$	(16) $\bar{y},x+\frac{1}{2},z+\frac{1}{2}$	
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}$	(18) $\bar{x},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{2},\bar{z},y+\frac{1}{2}$	
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}$	(22) $z+\frac{1}{2},\bar{y},x+\frac{1}{2}$	(23) $\bar{z},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z},\bar{y},\bar{x}$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(27) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(28) $\bar{x},y+\frac{1}{2},z+\frac{1}{2}$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x+\frac{1}{2},y+\frac{1}{2}$	(31) $z+\frac{1}{2},x+\frac{1}{2},\bar{y}$	(32) $z+\frac{1}{2},\bar{x},y+\frac{1}{2}$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{2},\bar{z},x+\frac{1}{2}$	(35) $\bar{y},z+\frac{1}{2},x+\frac{1}{2}$	(36) $y+\frac{1}{2},z+\frac{1}{2},\bar{x}$	
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(38) y,x,z	(39) $\bar{y}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	(40) $y,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y$	(42) $x,\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) x,z,y	(44) $\bar{x}+\frac{1}{2},z,\bar{y}+\frac{1}{2}$	
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x$	(46) $\bar{z}+\frac{1}{2},y,\bar{x}+\frac{1}{2}$	(47) $z,\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) z,y,x	
							Special: as above, plus
24	k	. . m	x,x,z	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,\bar{z}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	no extra conditions
			z,x,x	$z,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{z}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	
			x,z,x	$\bar{x}+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	$x,\bar{z}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},x$	
			$x+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x+\frac{1}{2},\bar{x},z+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},z+\frac{1}{2}$	
			$x+\frac{1}{2},z+\frac{1}{2},\bar{x}$	$\bar{x},z+\frac{1}{2},x+\frac{1}{2}$	$\bar{x},\bar{z},\bar{x}$	$x+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			$z+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$z+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{z},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{z},\bar{x},\bar{x}$	
24	j	. . 2	$\frac{1}{2},y,\bar{y}$	$0,\bar{y}+\frac{1}{2},\bar{y}$	$0,y,y+\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},y+\frac{1}{2}$	no extra conditions
			$\bar{y},\frac{1}{2},y$	$\bar{y},0,\bar{y}+\frac{1}{2}$	$y+\frac{1}{2},0,y$	$y+\frac{1}{2},\frac{1}{2},\bar{y}+\frac{1}{2}$	
			$y,\bar{y},\frac{1}{2}$	$\bar{y}+\frac{1}{2},\bar{y},0$	$y,y+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	
			$\frac{1}{2},\bar{y},y$	$0,y+\frac{1}{2},y$	$0,\bar{y},\bar{y}+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			$y,\frac{1}{2},\bar{y}$	$y,0,y+\frac{1}{2}$	$\bar{y}+\frac{1}{2},0,\bar{y}$	$\bar{y}+\frac{1}{2},\frac{1}{2},y+\frac{1}{2}$	
			$\bar{y},y,\frac{1}{2}$	$y+\frac{1}{2},y,0$	$\bar{y},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	
24	i	. . 2	$\frac{1}{2},y,y+\frac{1}{2}$	$0,\bar{y}+\frac{1}{2},y+\frac{1}{2}$	$0,y,\bar{y}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{y}$	no extra conditions
			$y+\frac{1}{2},\frac{1}{2},y$	$y+\frac{1}{2},0,\bar{y}+\frac{1}{2}$	$\bar{y},0,y$	$\bar{y},\frac{1}{2},\bar{y}+\frac{1}{2}$	
			$y,y+\frac{1}{2},\frac{1}{2}$	$\bar{y}+\frac{1}{2},y+\frac{1}{2},0$	$y,\bar{y},0$	$\bar{y}+\frac{1}{2},\bar{y},\frac{1}{2}$	
			$\frac{1}{2},\bar{y},\bar{y}+\frac{1}{2}$	$0,y+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0,\bar{y},y$	$\frac{1}{2},y+\frac{1}{2},y$	
			$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{y}$	$\bar{y}+\frac{1}{2},0,y+\frac{1}{2}$	$y,0,\bar{y}$	$y,\frac{1}{2},y+\frac{1}{2}$	
			$\bar{y},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},\bar{y}+\frac{1}{2},0$	$\bar{y},y,0$	$y+\frac{1}{2},y,\frac{1}{2}$	
24	h	2 . .	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},x$	$\frac{1}{4},\frac{3}{4},\bar{x}+\frac{1}{2}$	hkl: $h+k+l=2n$
			$\frac{3}{4},x+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},\bar{x},\frac{1}{4}$	$x+\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x+\frac{1}{2}$	
			$\bar{x},\frac{3}{4},\frac{1}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}$	$\frac{3}{4},\frac{1}{4},x+\frac{1}{2}$	
			$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},x,\frac{3}{4}$	$\bar{x}+\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$x,\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	
12	g	2 . mm	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x}+\frac{1}{2},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{1}{4},\frac{1}{4},\bar{x}+\frac{1}{2}$	hkl: $h+k+l=2n$
			$\frac{3}{4},x+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$x+\frac{1}{2},\frac{3}{4},\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{3}{4},\frac{3}{4},x+\frac{1}{2}$	
12	f	2 . 2 2	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},0,\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	hkl: $h+k+l=2n$
			$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{4},0$	
8	e	. 3 m	x,x,x	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$	$\bar{x}+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	no extra conditions
			$x+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},x+\frac{1}{2}$	
6	d	$\bar{4}$ 2 . m	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	hkl: $h+k+l=2n$
4	c	. $\bar{3}$ m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$			hkl: $h+k,h+l,k+l=2n$
4	b	. $\bar{3}$ m	$0,0,0$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $h+k,h+l,k+l=2n$
2	a	$\bar{4}$ 3 m	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl: $h+k+l=2n$



Symmetry of special projections

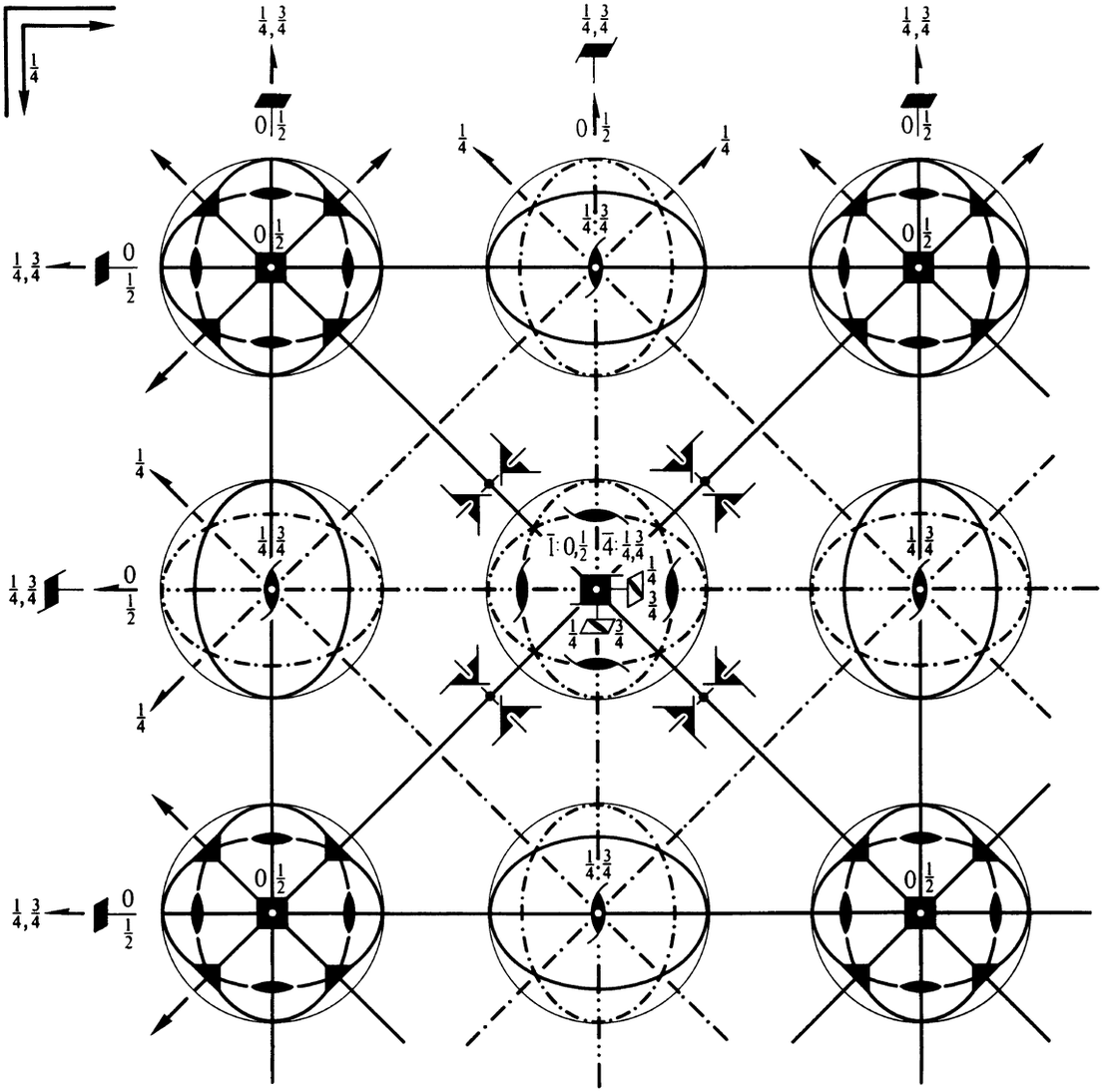
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{4},\frac{1}{4},z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

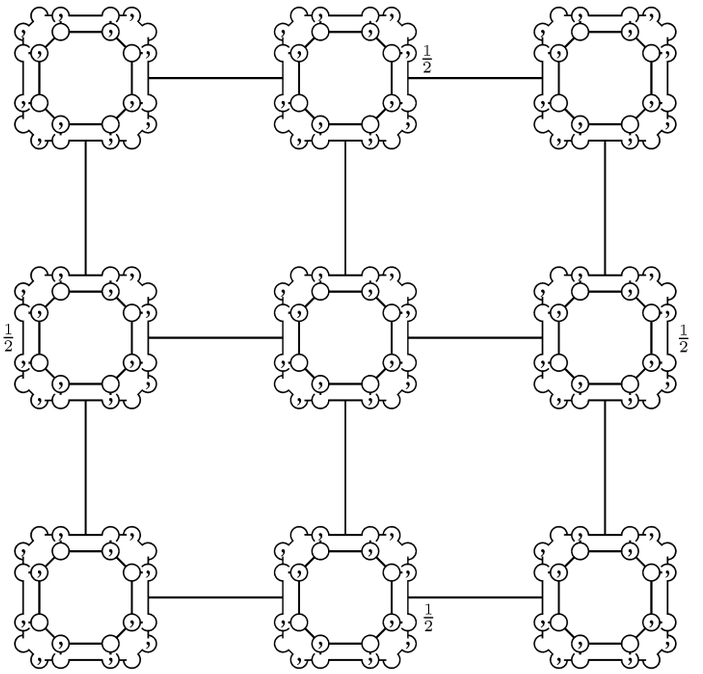
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$F\,m\bar{3}\,m$ O_h^5 $m\bar{3}\,m$ Cubic

No. 225 $F\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $F\,m\bar{3}\,m$



Upper left quadrant only



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Origin at centre $(m\bar{3}m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2}-x)$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
(2) 2 0,0,z
(3) 2 0,y,0
(4) 2 x,0,0
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x,\bar{x}$
(7) 3^+ $x,\bar{x},\bar{x}$
(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x},\bar{x}$
(11) 3^- $\bar{x},\bar{x},x$
(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 x,x,0
(14) 2 $x,\bar{x}$,0
(15) 4^- 0,0,z
(16) 4^+ 0,0,z
(17) 4^- x,0,0
(18) 2 0,y,y
(19) 2 0,$y,\bar{y}$
(20) 4^+ x,0,0
(21) 4^+ 0,y,0
(22) 2 x,0,x
(23) 4^- 0,y,0
(24) 2 $\bar{x}$,0,x
(25) $\bar{1}$ 0,0,0
(26) m x,y,0
(27) m x,0,z
(28) m 0,y,z
(29) $\bar{3}^+$ x,x,x; 0,0,0
(30) $\bar{3}^+$ $\bar{x},x,\bar{x}$; 0,0,0
(31) $\bar{3}^+$ $x,\bar{x},\bar{x}$; 0,0,0
(32) $\bar{3}^+$ $\bar{x},\bar{x},x$; 0,0,0
(33) $\bar{3}^-$ x,x,x; 0,0,0
(34) $\bar{3}^-$ $x,\bar{x},\bar{x}$; 0,0,0
(35) $\bar{3}^-$ $\bar{x},\bar{x},x$; 0,0,0
(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$; 0,0,0
(37) m $x,\bar{x},z$
(38) m x,x,z
(39) $\bar{4}^-$ 0,0,z; 0,0,0
(40) $\bar{4}^+$ 0,0,z; 0,0,0
(41) $\bar{4}^-$ x,0,0; 0,0,0
(42) m $x,y,\bar{y}$
(43) m x,y,y
(44) $\bar{4}^+$ x,0,0; 0,0,0
(45) $\bar{4}^+$ 0,y,0; 0,0,0
(46) m $\bar{x},y,x$
(47) $\bar{4}^-$ 0,y,0; 0,0,0
(48) m x,y,x

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$
(2) $2(0,0,\frac{1}{2})$ 0,$\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ 0,$y,\frac{1}{4}$
(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$
(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$
(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x+\frac{1}{4},\frac{1}{4}$
(14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{2})$ $-\frac{1}{4},\frac{1}{4},z$
(17) 4^- $x,\frac{1}{2},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ 0,y,y
(19) 2 0,$y+\frac{1}{2},\bar{y}$
(20) 4^+ x,0,$\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$
(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},\frac{1}{4},x$
(23) $4^-(0,\frac{1}{2},0)$ $-\frac{1}{4},y,\frac{1}{4}$
(24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}$ 0,$\frac{1}{4},\frac{1}{4}$
(26) b $x,y,\frac{1}{4}$
(27) c $x,\frac{1}{4},z$
(28) $n(0,\frac{1}{2},\frac{1}{2})$ 0,y,z
(29) $\bar{3}^+$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$
(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; $-\frac{1}{2},0,\frac{1}{2}$
(31) $\bar{3}^+$ $x,\bar{x}+\frac{1}{2},\bar{x}$; $0,\frac{1}{2},0$
(32) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{1}{2},0,\frac{1}{2}$
(33) $\bar{3}^-$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; $0,0,\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; $-\frac{1}{2},\frac{1}{2},0$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$
(37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x-\frac{1}{4},x,z$
(39) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^-$ x,0,$\frac{1}{2}$; 0,0,$\frac{1}{2}$
(42) m $x,y+\frac{1}{2},\bar{y}$
(43) $g(0,\frac{1}{2},\frac{1}{2})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{2},0$; $0,\frac{1}{2},0$
(45) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(46) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x-\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4}$,0,z
(3) 2 $\frac{1}{4},y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)$ x,0,$\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$
(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x-\frac{1}{4},\frac{1}{4}$
(14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{4},-\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(18) $2(0,\frac{1}{4},\frac{1}{2})$ $\frac{1}{4},y-\frac{1}{4},y$
(19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{1}{2},0,0)$ $x,-\frac{1}{4},\frac{1}{4}$
(21) 4^+ $\frac{1}{2},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ x,0,x
(23) 4^- 0,$y,\frac{1}{2}$
(24) 2 $\bar{x}+\frac{1}{2}$,0,x
(25) $\bar{1}$ $\frac{1}{4}$,0,$\frac{1}{4}$
(26) a $x,y,\frac{1}{4}$
(27) $n(\frac{1}{2},0,\frac{1}{2})$ x,0,z
(28) c $\frac{1}{4},y,z$
(29) $\bar{3}^+$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$; $0,0,\frac{1}{2}$
(31) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{1}{2},-\frac{1}{2},0$
(33) $\bar{3}^-$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-1,\bar{x}$; $0,-\frac{1}{2},\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x}+\frac{1}{2},\bar{x}+1,x$; $0,\frac{1}{2},\frac{1}{2}$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{1}{2},0,0$
(37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},x,z$
(39) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(42) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+$ 0,$y,\frac{1}{2}$; 0,0,$\frac{1}{2}$
(46) m $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{1}{2},y$,0; $\frac{1}{2}$,0,0
(48) $g(\frac{1}{2},0,\frac{1}{2})$ x,y,x

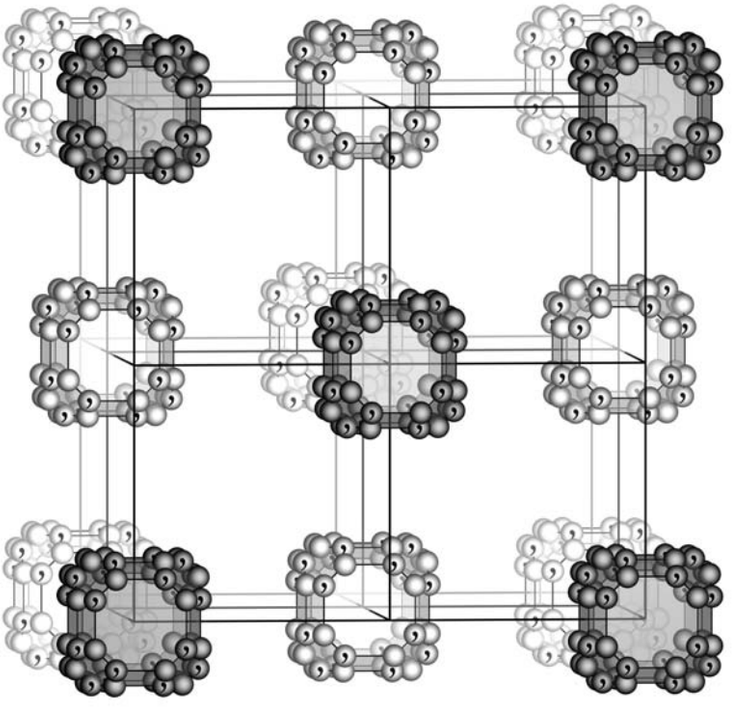
For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y$,0
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4}$,0
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$
(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$
(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ x,x,0
(14) 2 $x,\bar{x}+\frac{1}{2}$,0
(15) 4^- $\frac{1}{2}$,0,z
(16) 4^+ 0,$\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{4},-\frac{1}{4}$
(18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},y$
(19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{4},y,-\frac{1}{4}$
(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},\frac{1}{4},x$
(23) $4^-(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$
(24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4}$,0
(26) $n(\frac{1}{2},\frac{1}{2},0)$ x,y,0
(27) a $x,\frac{1}{4},z$
(28) b $\frac{1}{4},y,z$
(29) $\bar{3}^+$ $x+\frac{1}{2},x,x$; $\frac{1}{2}$,0,0
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; $0,\frac{1}{2},\frac{1}{2}$
(31) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+1,\bar{x}$; $0,\frac{1}{2},-\frac{1}{2}$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x},x$; $\frac{1}{2}$,0,0
(33) $\bar{3}^-$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2}$,0
(34) $\bar{3}^-$ $x+1,\bar{x}-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; $0,\frac{1}{2}$,0
(36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,-\frac{1}{2}$
(37) m $x+\frac{1}{2},\bar{x},z$
(38) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z
(39) $\bar{4}^-$ 0,$\frac{1}{2},z$; 0,$\frac{1}{2}$,0
(40) $\bar{4}^+$ $\frac{1}{2}$,0,z; $\frac{1}{2}$,0,0
(41) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(42) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(46) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x+\frac{1}{4},y,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates						Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$			h,k,l permutable General:
192	l	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $y,x,\bar{z}$ (17) $x,z,\bar{y}$ (21) $z,y,\bar{x}$ (25) $\bar{x},\bar{y},\bar{z}$ (29) $\bar{z},\bar{x},\bar{y}$ (33) $\bar{y},\bar{z},\bar{x}$ (37) $\bar{y},\bar{x},z$ (41) $\bar{x},\bar{z},y$ (45) $\bar{z},\bar{y},x$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $\bar{y},\bar{x},\bar{z}$ (18) $\bar{x},z,y$ (22) $z,\bar{y},x$ (26) $x,y,\bar{z}$ (30) $\bar{z},x,y$ (34) $y,\bar{z},x$ (38) y,x,z (42) $x,\bar{z},\bar{y}$ (46) $\bar{z},y,\bar{x}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $y,\bar{x},z$ (19) $\bar{x},\bar{z},\bar{y}$ (23) $\bar{z},y,x$ (27) $x,\bar{y},z$ (31) $z,x,\bar{y}$ (35) $\bar{y},z,x$ (39) $\bar{y},x,\bar{z}$ (43) x,z,y (47) $z,\bar{y},\bar{x}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{y},x,z$ (20) $x,\bar{z},y$ (24) $\bar{z},\bar{y},\bar{x}$ (28) $\bar{x},y,z$ (32) $z,\bar{x},y$ (36) $y,z,\bar{x}$ (40) $y,\bar{x},\bar{z}$ (44) $\bar{x},z,\bar{y}$ (48) z,y,x			hkl: $h+k,h+l,k+l=2n$ $0kl$: $k,l=2n$ hhl: $h+l=2n$ $h00$: $h=2n$
									Special: as above, plus
96	k	$..m$	x,x,z $\bar{z},\bar{x},x$ $x,x,\bar{z}$ $\bar{x},\bar{z},\bar{x}$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{z},x$	$\bar{x},x,\bar{z}$ x,z,x $x,\bar{x},z$ $z,x,\bar{x}$	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$ $\bar{x},x,z$ $z,\bar{x},x$	z,x,x $x,\bar{z},\bar{x}$ $x,z,\bar{x}$ $\bar{z},x,x$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$ $\bar{x},z,x$ $\bar{z},\bar{x},\bar{x}$	no extra conditions
96	j	$m..$	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$ $0,z,y$ $\bar{z},\bar{y},0$	no extra conditions
48	i	$m.m2$	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$	no extra conditions
48	h	$m.m2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$	no extra conditions
48	g	$2.mm$	$x,\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},x,\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x,\frac{1}{4}$ $x,\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$ $\bar{x},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$ $\frac{1}{4},\frac{1}{4},\bar{x}$	$\frac{3}{4},\frac{1}{4},\bar{x}$ $\frac{1}{4},\frac{3}{4},x$	hkl: $h=2n$
32	f	$.3\,m$	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$			no extra conditions
24	e	$4\,m\,.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
24	d	$m\,.\,mm$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h=2n$
8	c	$\bar{4}\,3\,m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$					hkl: $h=2n$
4	b	$m\bar{3}\,m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						no extra conditions
4	a	$m\bar{3}\,m$	$0,0,0$						no extra conditions



Symmetry of special projections

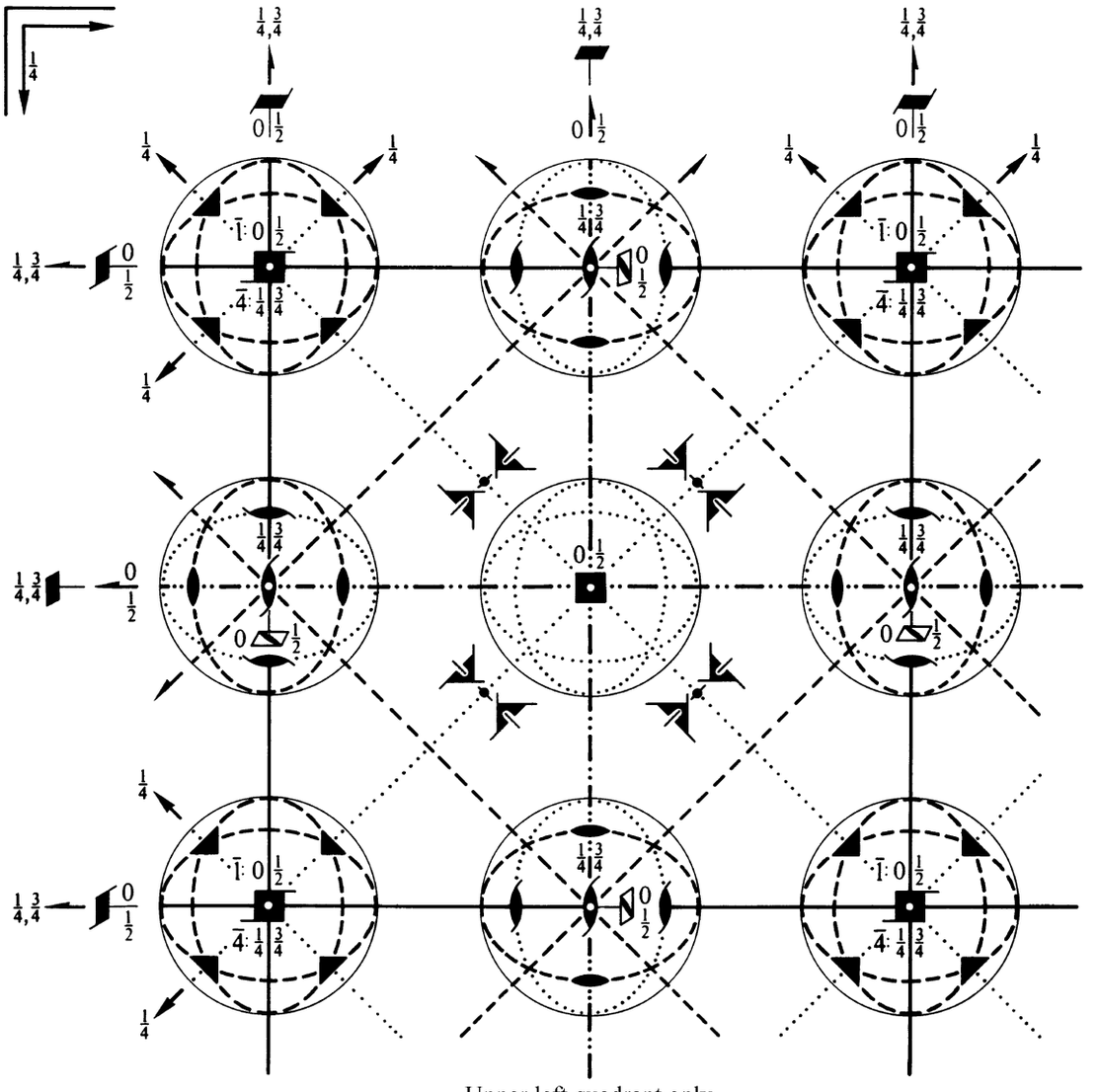
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

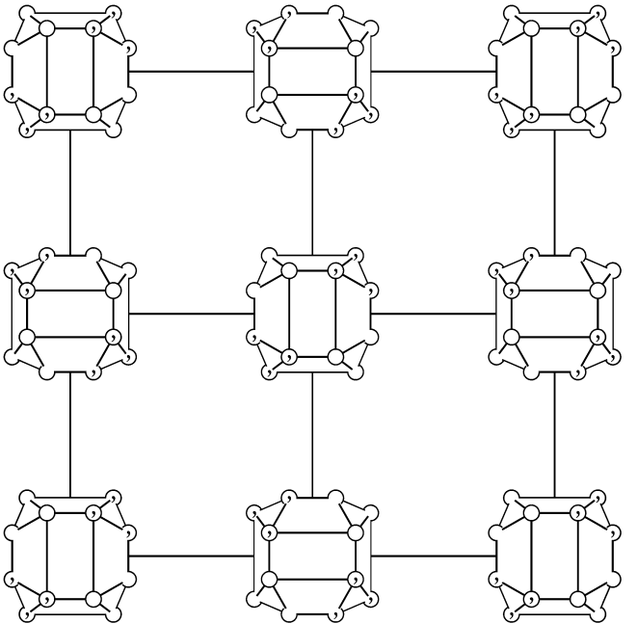
Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

$F\,m\bar{3}\,c$ O_h^6 $m\bar{3}m$ Cubic

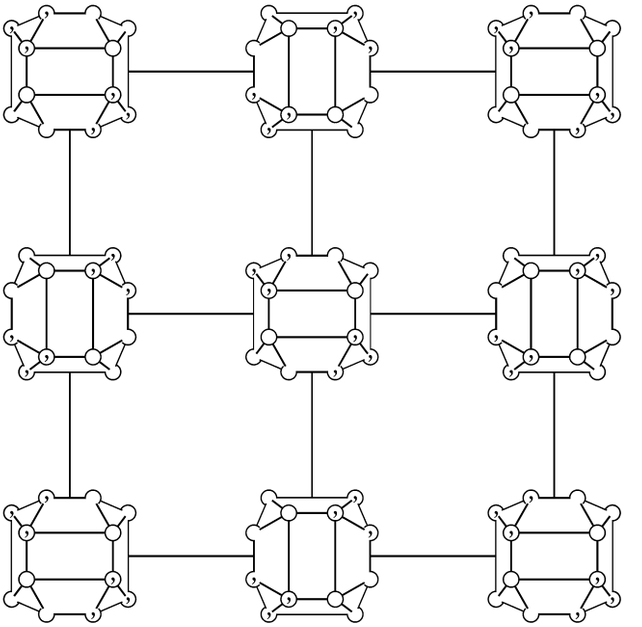
No. 226 $F\ 4/m\ \bar{3}\ 2/c$ Patterson symmetry $F\,m\bar{3}\,m$



Upper left quadrant only



Lower half of unit cell, all polyhedra at height 0



Upper half of unit cell, all polyhedra at height $\frac{1}{2}$

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Origin at centre $(m\bar{3})$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le \frac{1}{4}$; $y \le \min(x, \frac{1}{2}-x)$; $z \le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{4},\frac{1}{4},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
(2) 2 0,0,z
(3) 2 0,y,0
(4) 2 x,0,0
(5) 3^+ x,x,x
(6) 3^+ $\bar{x},x,\bar{x}$
(7) 3^+ $x,\bar{x},\bar{x}$
(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x},\bar{x}$
(11) 3^- $\bar{x},\bar{x},x$
(12) 3^- $\bar{x},x,\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$
(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2},0,z$
(16) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{2},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,y$
(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$
(20) $4^+(\frac{1}{2},0,0)$ $x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{2},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},x$
(23) $4^-(0,\frac{1}{2},0)$ $0,y,\frac{1}{2}$
(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}$ 0,0,0
(26) m $x,y,0$
(27) m $x,0,z$
(28) m $0,y,z$
(29) $\bar{3}^+$ x,x,x; 0,0,0
(30) $\bar{3}^+$ $\bar{x},x,\bar{x}$; 0,0,0
(31) $\bar{3}^+$ $x,\bar{x},\bar{x}$; 0,0,0
(32) $\bar{3}^+$ $\bar{x},\bar{x},x$; 0,0,0
(33) $\bar{3}^-$ x,x,x; 0,0,0
(34) $\bar{3}^-$ $x,\bar{x},\bar{x}$; 0,0,0
(35) $\bar{3}^-$ $\bar{x},\bar{x},x$; 0,0,0
(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$; 0,0,0
(37) c $x+\frac{1}{2},\bar{x},z$
(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z
(39) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^-$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$
(42) a $x,y+\frac{1}{2},\bar{y}$
(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$
(46) b $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$
(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$
(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$
(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$
(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$
(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x-\frac{1}{4},0$
(14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},0$
(15) 4^- $\frac{1}{4},-\frac{1}{4},z$
(16) 4^+ $\frac{1}{4},\frac{1}{4},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,0,0$
(18) 2 $\frac{1}{4},y,y$
(19) 2 $\frac{1}{4},y,\bar{y}$
(20) $4^+(\frac{1}{2},0,0)$ $x,0,0$
(21) 4^+ $\frac{1}{4},y,-\frac{1}{4}$
(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},0,x$
(23) 4^- $\frac{1}{4},y,\frac{1}{4}$
(24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},0,x$
(25) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$
(26) b $x,y,\frac{1}{4}$
(27) c $x,\frac{1}{4},z$
(28) $n(0,\frac{1}{2},\frac{1}{2})$ $0,y,z$
(29) $\bar{3}^+$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$
(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; $-\frac{1}{2},0,\frac{1}{2}$
(31) $\bar{3}^+$ $x,\bar{x}+\frac{1}{2},\bar{x}$; $0,\frac{1}{2},0$
(32) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{1}{2},0,\frac{1}{2}$
(33) $\bar{3}^-$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; $0,0,\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; $-\frac{1}{2},\frac{1}{2},0$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$
(37) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$
(39) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$
(40) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$
(41) $\bar{4}^-$ $x,0,0$; $\frac{1}{4},0,0$
(42) a $x,y,\bar{y}$
(43) a x,y,y
(44) $\bar{4}^+$ $x,0,0$; $\frac{1}{4},0,0$
(45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$
(46) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},0,-\frac{1}{4}$
(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(3) 2 $\frac{1}{4},y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$
(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x+\frac{1}{4},0$
(14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},0$
(15) 4^- $\frac{1}{4},\frac{1}{4},z$
(16) 4^+ $-\frac{1}{4},\frac{1}{4},z$
(17) 4^- $x,\frac{1}{4},-\frac{1}{4}$
(18) $2(0,\frac{1}{4},\frac{1}{4})$ $0,y+\frac{1}{4},y$
(19) $2(0,\frac{1}{4},-\frac{1}{4})$ $0,y+\frac{1}{4},\bar{y}$
(20) 4^+ $x,\frac{1}{4},\frac{1}{4}$
(21) $4^+(0,\frac{1}{2},0)$ $0,y,0$
(22) 2 $x,\frac{1}{4},x$
(23) $4^-(0,\frac{1}{2},0)$ $0,y,0$
(24) 2 $\bar{x},\frac{1}{4},x$
(25) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$
(26) a $x,y,\frac{1}{4}$
(27) $n(\frac{1}{2},0,\frac{1}{2})$ $x,0,z$
(28) c $\frac{1}{4},y,z$
(29) $\bar{3}^+$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$; $0,0,\frac{1}{2}$
(31) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{1}{2},-\frac{1}{2},0$
(33) $\bar{3}^-$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-1,\bar{x}$; $0,-\frac{1}{2},\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x}+\frac{1}{2},\bar{x}+1,x$; $0,\frac{1}{2},\frac{1}{2}$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{1}{2},0,0$
(37) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$
(39) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$
(40) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$
(41) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$
(42) $g(0,\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}$; $0,\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^+$ $0,y,0$; $0,\frac{1}{4},0$
(46) b $\bar{x},y,x$
(47) $\bar{4}^-$ $0,y,0$; $0,\frac{1}{4},0$
(48) b x,y,x

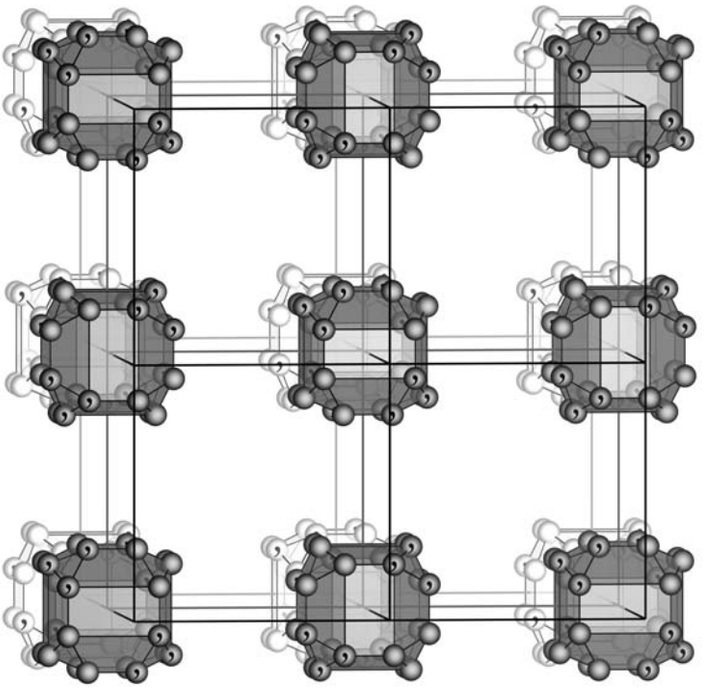
For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$
(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$
(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) 2 $x,x,\frac{1}{4}$
(14) 2 $x,\bar{x},\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{2})$ $0,0,z$
(16) $4^+(0,0,\frac{1}{2})$ $0,0,z$
(17) 4^- $x,\frac{1}{4},\frac{1}{4}$
(18) $2(0,\frac{1}{4},\frac{1}{4})$ $0,y-\frac{1}{4},y$
(19) $2(0,-\frac{1}{4},\frac{1}{4})$ $0,y+\frac{1}{4},\bar{y}$
(20) 4^+ $x,-\frac{1}{4},\frac{1}{4}$
(21) 4^+ $\frac{1}{4},y,\frac{1}{4}$
(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},0,x$
(23) 4^- $-\frac{1}{4},y,\frac{1}{4}$
(24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},0,x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
(26) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,0$
(27) a $x,\frac{1}{4},z$
(28) b $\frac{1}{4},y,z$
(29) $\bar{3}^+$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; $0,\frac{1}{2},\frac{1}{2}$
(31) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+1,\bar{x}$; $0,\frac{1}{2},-\frac{1}{2}$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x},x$; $\frac{1}{2},0,0$
(33) $\bar{3}^-$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$
(34) $\bar{3}^-$ $x+1,\bar{x}-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; $0,\frac{1}{2},0$
(36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{1}{2},0,-\frac{1}{2}$
(37) c $x,\bar{x},z$
(38) c x,x,z
(39) $\bar{4}^-$ $0,0,z$; $0,0,\frac{1}{4}$
(40) $\bar{4}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(41) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}$; $0,-\frac{1}{4},\frac{1}{4}$
(42) $g(0,-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},0,\frac{1}{4}$
(46) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$
(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$			Reflection conditions
									h,k,l permutable
									General:
192	j	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$			hkl: $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$			$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$			hhl: $h,l=2n$
			(13) $y+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$			$h00$: $h=2n$
			(17) $x+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$			
			(21) $z+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{z}+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$			
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$			
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$			
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$			
			(37) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$			
			(41) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$			
			(45) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},x+\frac{1}{2}$	(46) $\bar{z}+\frac{1}{2},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$			
									Special: as above, plus
96	i	$m\,.\,.$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$			no extra conditions
			$z,0,y$	$z,0,\bar{y}$	$\bar{z},0,y$	$\bar{z},0,\bar{y}$			
			$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$			
			$y+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$y+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\bar{y}+\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$			
			$\frac{1}{2},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	$\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	$\frac{1}{2},\bar{z}+\frac{1}{2},y+\frac{1}{2}$			
			$z+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$z+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$\bar{z}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$			
96	h	$\,.\,.2$	$\frac{1}{4},y,y$	$\frac{3}{4},\bar{y},y$	$\frac{3}{4},y,\bar{y}$	$\frac{1}{4},\bar{y},\bar{y}$	$y,\frac{1}{4},y$	$y,\frac{3}{4},\bar{y}$	hkl: $h=2n$
			$\bar{y},\frac{3}{4},y$	$\bar{y},\frac{1}{4},\bar{y}$	$y,y,\frac{1}{4}$	$\bar{y},y,\frac{3}{4}$	$y,\bar{y},\frac{3}{4}$	$\bar{y},\bar{y},\frac{1}{4}$	
			$\frac{3}{4},\bar{y},\bar{y}$	$\frac{1}{4},y,\bar{y}$	$\frac{1}{4},\bar{y},y$	$\frac{3}{4},y,y$	$\bar{y},\frac{3}{4},\bar{y}$	$\bar{y},\frac{1}{4},y$	
			$y,\frac{1}{4},\bar{y}$	$y,\frac{3}{4},y$	$\bar{y},\bar{y},\frac{3}{4}$	$y,\bar{y},\frac{1}{4}$	$\bar{y},y,\frac{1}{4}$	$y,y,\frac{3}{4}$	
64	g	$.\,3\,.$	x,x,x	$\bar{x},\bar{x},x$					hkl: $h=2n$
			$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$					
			$x+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$					
			$x+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
			$\bar{x},\bar{x},\bar{x}$	$x,x,\bar{x}$					
			$x,\bar{x},x$	$\bar{x},x,x$					
			$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$					
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$					
48	f	$4\,.\,.$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	hkl: $h=2n$
			$\bar{x},\frac{3}{4},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{3}{4},x,\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x$	
48	e	$m\,m\,2\,.\,.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$			hkl: $h=2n$
			$0,0,x$	$0,0,\bar{x}$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$			
			$x+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{x}+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x+\frac{1}{2}$			
24	d	$4/m\,.\,.$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$	hkl: $h=2n$
24	c	$\bar{4}\,m\,.\,2$	$\frac{1}{4},0,0$	$\frac{3}{4},0,0$	$0,\frac{1}{4},0$	$0,\frac{3}{4},0$	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$	hkl: $h=2n$
8	b	$m\,\bar{3}\,.$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					hkl: $h=2n$
8	a	$4\,3\,2$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					hkl: $h=2n$



Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $0,0,z$

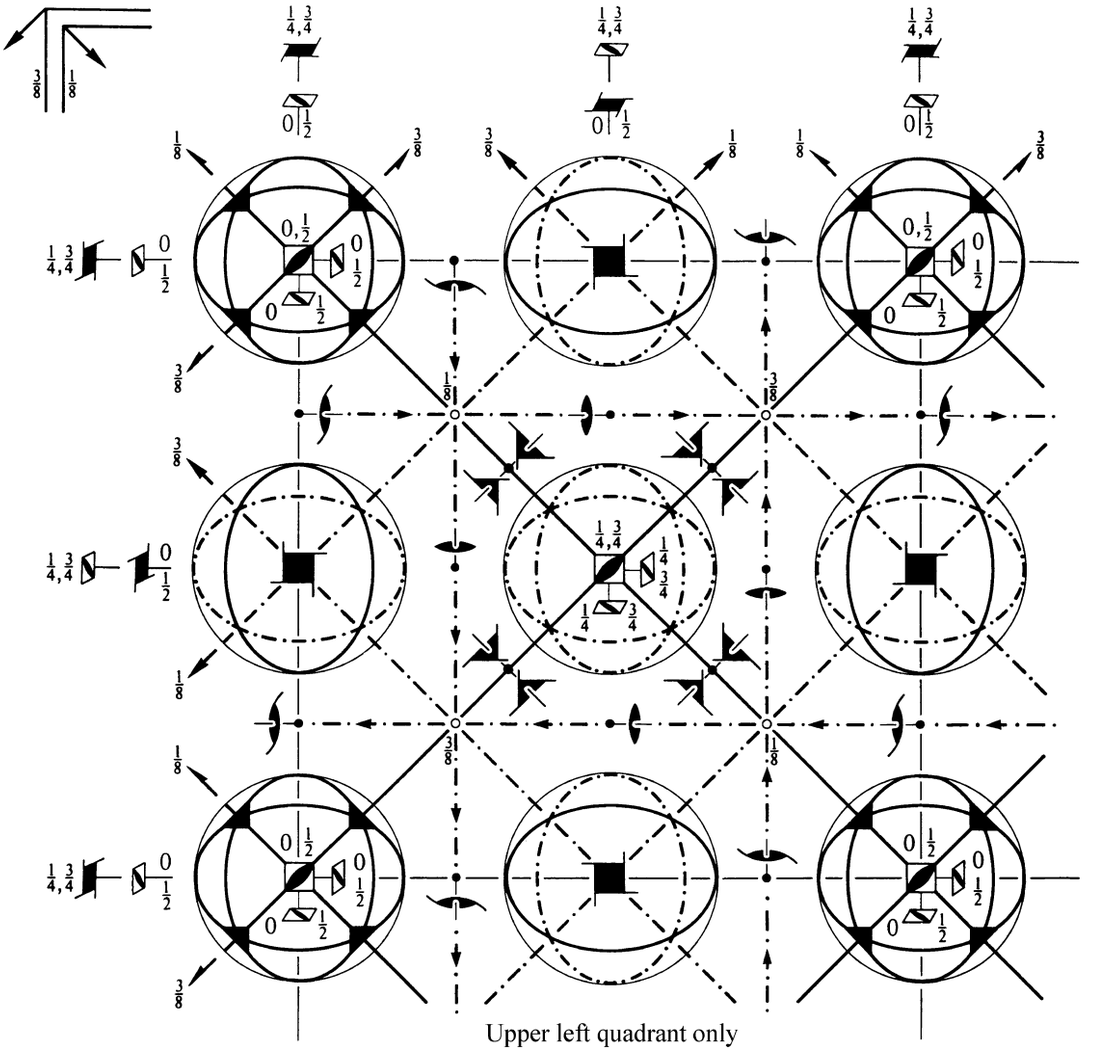
Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

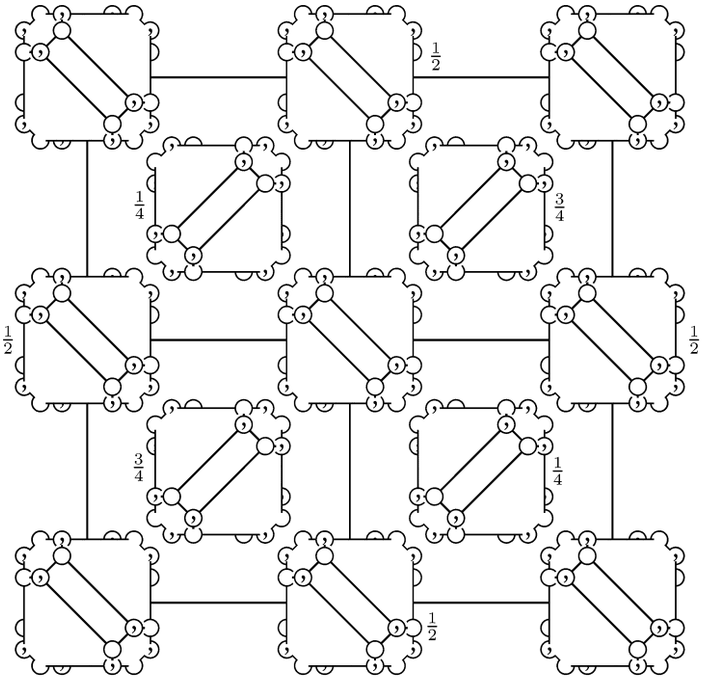
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$F\,d\,\bar{3}\,m$ O_h^7 $m\,\bar{3}\,m$ Cubic

No. 227 $F\ 4_1/d\ \bar{3}\ 2/m$ Patterson symmetry $F\,m\,\bar{3}\,m$

ORIGIN CHOICE 1





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Origin at $\bar{4}\,3\,m$, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre $(\bar{3}\,m)$

Asymmetric unit $0\le x\le\frac{1}{2};\quad 0\le y\le\frac{1}{8};\quad -\frac{1}{8}\le z\le\frac{1}{8};\quad y\le\min(\frac{1}{2}-x,x);\quad -y\le z\le y$

Vertices $0,0,0\quad\frac{1}{2},0,0\quad\frac{3}{8},\frac{1}{8},\frac{1}{8}\quad\frac{1}{8},\frac{1}{8},\frac{1}{8}\quad\frac{3}{8},\frac{1}{8},-\frac{1}{8}\quad\frac{1}{8},\frac{1}{8},-\frac{1}{8}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
(2) $2(0,0,\frac{1}{2})\quad 0,\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,0$
(4) $2(\frac{1}{2},0,0)\quad x,0,\frac{1}{4}$
(5) $3^+\quad x,x,x$
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) $3^-\quad x,x,x$
(10) $3^-\quad x,\bar{x}+\frac{1}{2},\bar{x}$
(11) $3^-\quad \bar{x}+\frac{1}{2},\bar{x},x$
(12) $3^-\quad \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x-\frac{1}{4},\frac{3}{8}$
(14) $2\quad x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{3}{4})\quad \frac{1}{2},\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{4})\quad 0,\frac{3}{4},z$
(17) $4^-(\frac{3}{4},0,0)\quad x,\frac{1}{2},\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{3}{8},y+\frac{1}{4},y$
(19) $2\quad \frac{1}{8},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)\quad x,0,\frac{3}{4}$
(21) $4^+(0,\frac{1}{4},0)\quad \frac{3}{4},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x-\frac{1}{4},\frac{3}{8},x$
(23) $4^-(0,\frac{3}{4},0)\quad \frac{1}{4},y,\frac{1}{2}$
(24) $2\quad \bar{x}+\frac{1}{4},\frac{1}{8},x$
(25) $\bar{1}\quad \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(26) $d(\frac{1}{4},\frac{3}{4},0)\quad x,y,\frac{3}{8}$
(27) $d(\frac{3}{4},0,\frac{1}{4})\quad x,\frac{3}{8},z$
(28) $d(0,\frac{1}{4},\frac{3}{4})\quad \frac{3}{8},y,z$
(29) $\bar{3}^+\quad x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(30) $\bar{3}^+\quad \bar{x}-1,x+1,\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{7}{8}$
(31) $\bar{3}^+\quad x,\bar{x}+1,\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{1}{8}$
(32) $\bar{3}^+\quad \bar{x}+1,\bar{x},x;\ \frac{7}{8},-\frac{1}{8},\frac{1}{8}$
(33) $\bar{3}^-\quad x,x,x;\ \frac{1}{8},\frac{1}{8},\frac{1}{8}$
(34) $\bar{3}^-\quad x+\frac{3}{2},\bar{x}-1,\bar{x};\ \frac{5}{8},-\frac{1}{8},\frac{7}{8}$
(35) $\bar{3}^-\quad \bar{x}+\frac{1}{2},\bar{x}+\frac{3}{2},x;\ -\frac{1}{8},\frac{7}{8},\frac{5}{8}$
(36) $\bar{3}^-\quad \bar{x}+1,x+\frac{1}{2},\bar{x};\ \frac{7}{8},\frac{5}{8},-\frac{1}{8}$
(37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},\bar{x},z$
(38) $m\quad x,x,z$
(39) $4^-\quad -\frac{1}{4},\frac{1}{4},z;\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(40) $\bar{4}^+\quad \frac{1}{2},0,z;\ \frac{1}{2},0,0$
(41) $\bar{4}^-\quad x,-\frac{1}{4},\frac{1}{4};\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(42) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$
(43) $m\quad x,y,y$
(44) $\bar{4}^+\quad x,\frac{1}{2},0;\ 0,\frac{1}{2},0$
(45) $\bar{4}^+\quad 0,y,\frac{1}{2};\ 0,0,\frac{1}{2}$
(46) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-\quad \frac{1}{4},y,-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(48) $m\quad x,y,x$

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$
(2) $2\quad 0,0,z$
(3) $2\quad \frac{1}{4},y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{3},x-\frac{1}{6},x$
(6) $3^+\quad \bar{x}+\frac{1}{2},x,\bar{x}$
(7) $3^+\quad x,\bar{x},\bar{x}$
(8) $3^+\quad \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x+\frac{1}{6},x$
(10) $3^-\quad x+\frac{1}{2},\bar{x},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})\quad \bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^-\quad \bar{x},x,\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)\quad x,x,\frac{1}{8}$
(14) $2(-\frac{1}{4},\frac{1}{4},0)\quad x,\bar{x}+\frac{1}{2},\frac{3}{8}$
(15) $4^-(0,0,\frac{1}{4})\quad \frac{1}{4},0,z$
(16) $4^+(0,0,\frac{3}{4})\quad \frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{3}{4},0,0)\quad x,\frac{1}{2},-\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})\quad \frac{3}{8},y-\frac{1}{4},y$
(19) $2\quad \frac{1}{8},y+\frac{3}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)\quad x,0,\frac{1}{4}$
(21) $4^+(0,\frac{3}{4},0)\quad \frac{1}{2},y,-\frac{1}{4}$
(22) $2(\frac{1}{4},0,\frac{1}{4})\quad x,\frac{1}{8},x$
(23) $4^-(0,\frac{1}{4},0)\quad 0,y,\frac{3}{4}$
(24) $2(-\frac{1}{4},0,\frac{1}{4})\quad \bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}\quad \frac{1}{8},\frac{3}{8},\frac{3}{8}$
(26) $d(\frac{1}{4},\frac{1}{4},0)\quad x,y,\frac{1}{8}$
(27) $d(\frac{3}{4},0,\frac{3}{4})\quad x,\frac{1}{8},z$
(28) $d(0,\frac{3}{4},\frac{1}{4})\quad \frac{3}{8},y,z$
(29) $\bar{3}^+\quad x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$
(30) $\bar{3}^+\quad \bar{x}-1,x+\frac{3}{2},\bar{x};\ -\frac{1}{8},\frac{5}{8},\frac{7}{8}$
(31) $\bar{3}^+\quad x,\bar{x}+\frac{1}{2},\bar{x};\ \frac{1}{8},\frac{3}{8},-\frac{1}{8}$
(32) $\bar{3}^+\quad \bar{x}+1,\bar{x}-\frac{1}{2},x;\ \frac{7}{8},-\frac{5}{8},\frac{1}{8}$
(33) $\bar{3}^-\quad x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$
(34) $\bar{3}^-\quad x+1,\bar{x}-\frac{3}{2},\bar{x};\ \frac{1}{8},-\frac{5}{8},\frac{7}{8}$
(35) $\bar{3}^-\quad \bar{x},\bar{x}+1,x;\ -\frac{1}{8},\frac{7}{8},\frac{1}{8}$
(36) $\bar{3}^-\quad \bar{x}+\frac{1}{2},x,\bar{x};\ \frac{3}{8},\frac{1}{8},-\frac{1}{8}$
(37) $m\quad x+\frac{1}{2},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x-\frac{1}{4},x,z$
(39) $\bar{4}^-\quad 0,0,z;\ 0,0,0$
(40) $\bar{4}^+\quad \frac{1}{4},-\frac{1}{4},z;\ \frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^-\quad x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(42) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},\bar{y}$
(43) $g(0,\frac{1}{2},\frac{1}{2})\quad x,y,y$
(44) $\bar{4}^+\quad x,0,0;\ 0,0,0$
(45) $\bar{4}^+\quad \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(46) $m\quad \bar{x},y,x$
(47) $\bar{4}^-\quad \frac{1}{2},y,0;\ \frac{1}{2},0,0$
(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})\quad x-\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$
(2) $2\quad \frac{1}{4},\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)\quad 0,y,\frac{1}{4}$
(4) $2\quad x,0,0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x-\frac{1}{6},x$
(6) $3^+\quad \bar{x},x,\bar{x}$
(7) $3^+\quad x+\frac{1}{2},\bar{x},\bar{x}$
(8) $3^+\quad \bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x-\frac{1}{6},x-\frac{1}{3},x$
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^-\quad \bar{x},\bar{x},x$
(12) $3^-\quad \bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)\quad x,x,\frac{1}{8}$
(14) $2(\frac{1}{4},-\frac{1}{4},0)\quad x,\bar{x}+\frac{1}{2},\frac{3}{8}$
(15) $4^-(0,0,\frac{1}{4})\quad \frac{3}{4},0,z$
(16) $4^+(0,0,\frac{3}{4})\quad -\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)\quad x,\frac{1}{4},0$
(18) $2(0,\frac{3}{4},\frac{3}{4})\quad \frac{1}{8},y,y$
(19) $2(0,-\frac{1}{4},\frac{1}{4})\quad \frac{3}{8},y+\frac{1}{2},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)\quad x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)\quad \frac{1}{4},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})\quad x+\frac{1}{4},\frac{3}{8},x$
(23) $4^-(0,\frac{3}{4},0)\quad -\frac{1}{4},y,\frac{1}{2}$
(24) $2\quad \bar{x}+\frac{3}{4},\frac{1}{8},x$
(25) $\bar{1}\quad \frac{3}{8},\frac{1}{8},\frac{3}{8}$
(26) $d(\frac{3}{4},\frac{3}{4},0)\quad x,y,\frac{1}{8}$
(27) $d(\frac{1}{4},0,\frac{3}{4})\quad x,\frac{3}{8},z$
(28) $d(0,\frac{1}{4},\frac{1}{4})\quad \frac{1}{8},y,z$
(29) $\bar{3}^+\quad x-\frac{1}{2},x-\frac{1}{2},x;\ \frac{1}{8},\frac{1}{8},\frac{5}{8}$
(30) $\bar{3}^+\quad \bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x};\ -\frac{1}{8},\frac{1}{8},\frac{3}{8}$
(31) $\bar{3}^+\quad x-\frac{1}{2},\bar{x}+\frac{3}{2},\bar{x};\ \frac{1}{8},\frac{7}{8},-\frac{5}{8}$
(32) $\bar{3}^+\quad \bar{x}+\frac{3}{2},\bar{x}+\frac{1}{2},x;\ \frac{7}{8},-\frac{1}{8},\frac{5}{8}$
(33) $\bar{3}^-\quad x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$
(34) $\bar{3}^-\quad x+1,\bar{x}-1,\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{7}{8}$
(35) $\bar{3}^-\quad \bar{x},\bar{x}+\frac{1}{2},x;\ -\frac{1}{8},\frac{3}{8},\frac{1}{8}$
(36) $\bar{3}^-\quad \bar{x}+\frac{3}{2},x-\frac{1}{2},\bar{x};\ \frac{7}{8},\frac{1}{8},-\frac{5}{8}$
(37) $m\quad x,\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},x,z$
(39) $\bar{4}^-\quad 0,\frac{1}{2},z;\ 0,\frac{1}{2},0$
(40) $\bar{4}^+\quad \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(41) $\bar{4}^-\quad x,0,0;\ 0,0,0$
(42) $m\quad x,y+\frac{1}{2},\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y-\frac{1}{4},y$
(44) $\bar{4}^+\quad x,\frac{1}{4},-\frac{1}{4};\ \frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^+\quad 0,y,0;\ 0,0,0$
(46) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})\quad \bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-\quad \frac{1}{4},y,\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(48) $g(\frac{1}{2},0,\frac{1}{2})\quad x,y,x$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

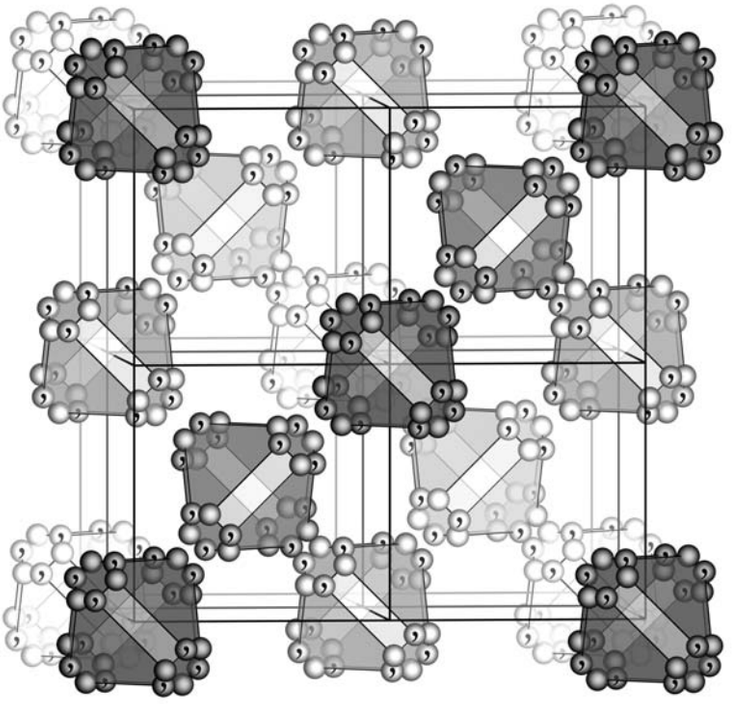
(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) $2(0,0,\frac{1}{2})\quad \frac{1}{4},0,z$
(3) $2\quad 0,y,0$
(4) $2\quad x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{6},x+\frac{1}{3},x$
(6) $3^+\quad \bar{x},x+\frac{1}{2},\bar{x}$
(7) $3^+\quad x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) $3^+\quad \bar{x},\bar{x},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})\quad x+\frac{1}{3},x+\frac{1}{6},x$
(10) $3^-\quad x,\bar{x},\bar{x}$
(11) $3^-\quad \bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})\quad \bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)\quad x,x+\frac{1}{4},\frac{3}{8}$
(14) $2\quad x,\bar{x}+\frac{3}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{3}{4})\quad \frac{1}{2},-\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{4})\quad 0,\frac{1}{4},z$
(17) $4^-(\frac{1}{4},0,0)\quad x,\frac{3}{4},0$
(18) $2(0,\frac{1}{4},\frac{1}{4})\quad \frac{1}{8},y,y$
(19) $2(0,\frac{1}{4},-\frac{1}{4})\quad \frac{3}{8},y+\frac{1}{2},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)\quad x,-\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)\quad \frac{1}{2},y,\frac{1}{4}$
(22) $2(\frac{3}{4},0,\frac{3}{4})\quad x,\frac{1}{8},x$
(23) $4^-(0,\frac{1}{4},0)\quad 0,y,\frac{1}{4}$
(24) $2(\frac{1}{4},0,-\frac{1}{4})\quad \bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}\quad \frac{3}{8},\frac{3}{8},\frac{1}{8}$
(26) $d(\frac{3}{4},\frac{1}{4},0)\quad x,y,\frac{3}{8}$
(27) $d(\frac{1}{4},0,\frac{1}{4})\quad x,\frac{1}{8},z$
(28) $d(0,\frac{3}{4},\frac{3}{4})\quad \frac{1}{8},y,z$
(29) $\bar{3}^+\quad x+\frac{1}{2},x,x;\ \frac{5}{8},\frac{1}{8},\frac{1}{8}$
(30) $\bar{3}^+\quad \bar{x}-\frac{3}{2},x+1,\bar{x};\ -\frac{5}{8},\frac{1}{8},\frac{7}{8}$
(31) $\bar{3}^+\quad x+\frac{1}{2},\bar{x}+1,\bar{x};\ \frac{5}{8},\frac{7}{8},-\frac{1}{8}$
(32) $\bar{3}^+\quad \bar{x}+\frac{1}{2},\bar{x},x;\ \frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(33) $\bar{3}^-\quad x,x+\frac{1}{2},x;\ \frac{1}{8},\frac{5}{8},\frac{1}{8}$
(34) $\bar{3}^-\quad x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x};\ \frac{1}{8},-\frac{1}{8},\frac{3}{8}$
(35) $\bar{3}^-\quad \bar{x}-\frac{1}{2},\bar{x}+1,x;\ -\frac{5}{8},\frac{7}{8},\frac{1}{8}$
(36) $\bar{3}^-\quad \bar{x}+1,x,\bar{x};\ \frac{7}{8},\frac{1}{8},-\frac{1}{8}$
(37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})\quad x+\frac{1}{4},\bar{x},z$
(38) $g(\frac{1}{2},\frac{1}{2},0)\quad x,x,z$
(39) $\bar{4}^-\quad \frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(40) $\bar{4}^+\quad 0,0,z;\ 0,0,0$
(41) $\bar{4}^-\quad x,0,\frac{1}{2};\ 0,0,\frac{1}{2}$
(42) $m\quad x,y,\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})\quad x,y+\frac{1}{4},y$
(44) $\bar{4}^+\quad x,\frac{1}{4},\frac{1}{4};\ \frac{1}{4},\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+\quad -\frac{1}{4},y,\frac{1}{4};\ -\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(46) $m\quad \bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-\quad 0,y,0;\ 0,0,0$
(48) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})\quad x+\frac{1}{4},y,x$

ORIGIN CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							h,k,l permutable
							General:
192	i	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$	$0kl$: $k+l=4n$ and $k,l=2n$
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	hhl: $h+l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	$h00$: $h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
			(25) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{3}{4}$	(27) $x+\frac{3}{4},\bar{y}+\frac{3}{4},z+\frac{1}{4}$	(28) $\bar{x}+\frac{3}{4},y+\frac{1}{4},z+\frac{3}{4}$	
			(29) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(30) $\bar{z}+\frac{3}{4},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{3}{4}$	(32) $z+\frac{3}{4},\bar{x}+\frac{3}{4},y+\frac{1}{4}$	
			(33) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	(34) $y+\frac{3}{4},\bar{z}+\frac{3}{4},x+\frac{1}{4}$	(35) $\bar{y}+\frac{3}{4},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{3}{4}$	
			(37) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$	
			(41) $\bar{x}+\frac{1}{2},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}$	(43) x,z,y	(44) $\bar{x},z+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(45) $\bar{z}+\frac{1}{2},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}$	(48) z,y,x	
							Special: as above, plus
96	h	. . 2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{7}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{5}{8},\bar{y},y+\frac{1}{4}$	no extra conditions
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{7}{8},\bar{y}+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{8},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{5}{8},\bar{y}$	
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{7}{8}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{3}{8}$	$\bar{y},y+\frac{1}{4},\frac{5}{8}$	
			$\frac{1}{8},\bar{y}+\frac{1}{4},y$	$\frac{3}{8},y+\frac{3}{4},y+\frac{1}{2}$	$\frac{7}{8},\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2}$	$\frac{5}{8},y+\frac{1}{4},\bar{y}$	
			$y,\frac{1}{8},\bar{y}+\frac{1}{4}$	$y+\frac{1}{2},\frac{3}{8},y+\frac{3}{4}$	$\bar{y}+\frac{1}{2},\frac{7}{8},\bar{y}+\frac{3}{4}$	$\bar{y},\frac{5}{8},y+\frac{1}{4}$	
			$\bar{y}+\frac{1}{4},y,\frac{1}{8}$	$y+\frac{3}{4},y+\frac{1}{2},\frac{3}{8}$	$\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2},\frac{7}{8}$	$y+\frac{1}{4},\bar{y},\frac{5}{8}$	
96	g	. . m	x,x,z	$\bar{x},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$	no extra conditions
			z,x,x	$z+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$	$\bar{z},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	
			x,z,x	$\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	
			$x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	
			$x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{3}{4},z+\frac{3}{4},x+\frac{1}{4}$	$\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{z}+\frac{3}{4},x+\frac{3}{4}$	
			$z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$z+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{z}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$	$\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
48	f	2 . mm	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$0,x,0$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$0,0,x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	hkl: $h=2n+1$ or $h+k+l=4n$
			$\frac{3}{4},x+\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},x+\frac{3}{4}$	
32	e	. 3 m	x,x,x	$\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$					no extra conditions
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$					
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$					
			$x+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$					
16	d	. $\bar{3}$ m	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{7}{8}$			hkl: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	. $\bar{3}$ m	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{3}{8}$			
8	b	$\bar{4}$ 3 m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$					hkl: $h=2n+1$ or $h+k+l=4n$
8	a	$\bar{4}$ 3 m	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$					



Symmetry of special projections

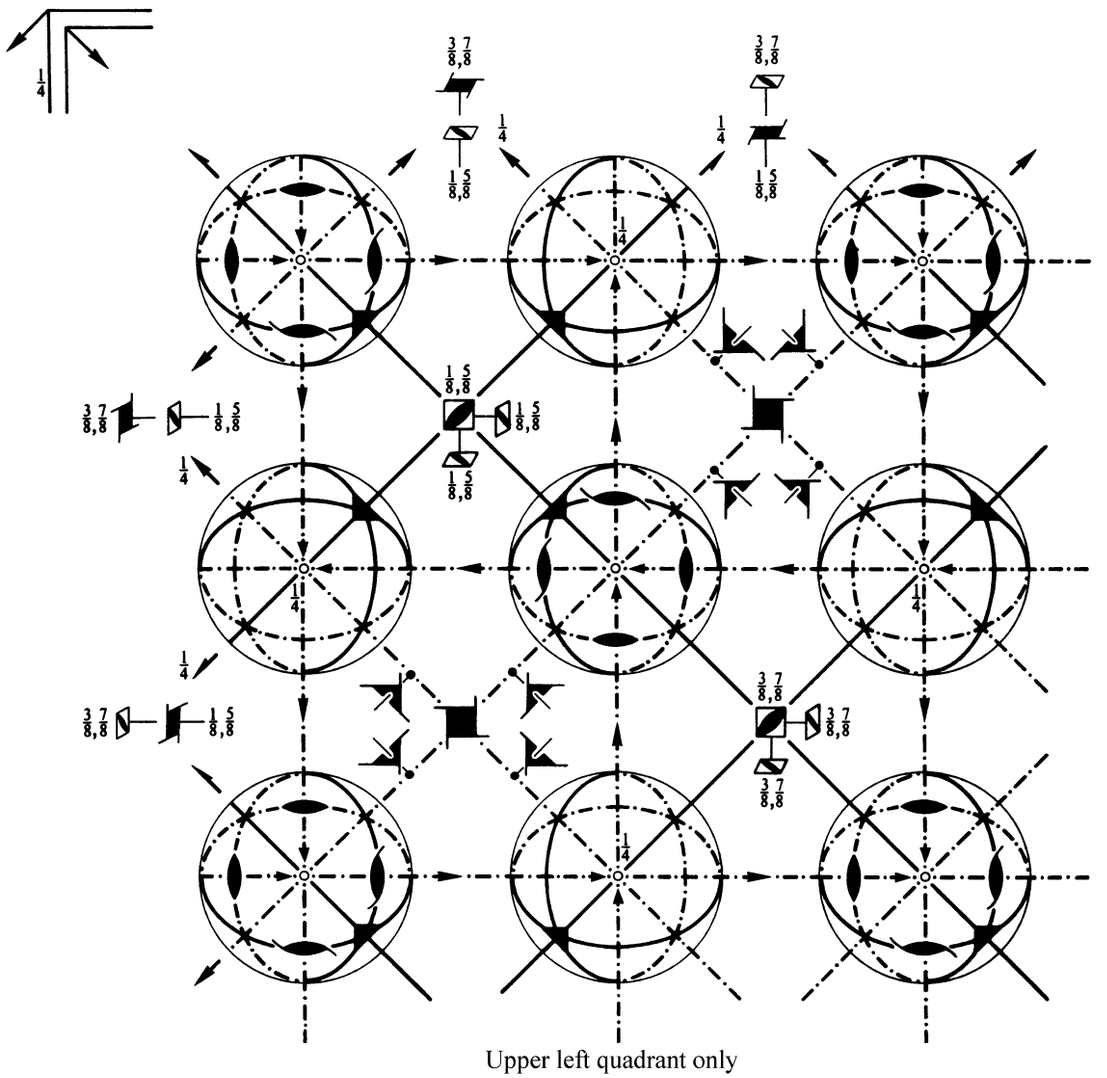
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

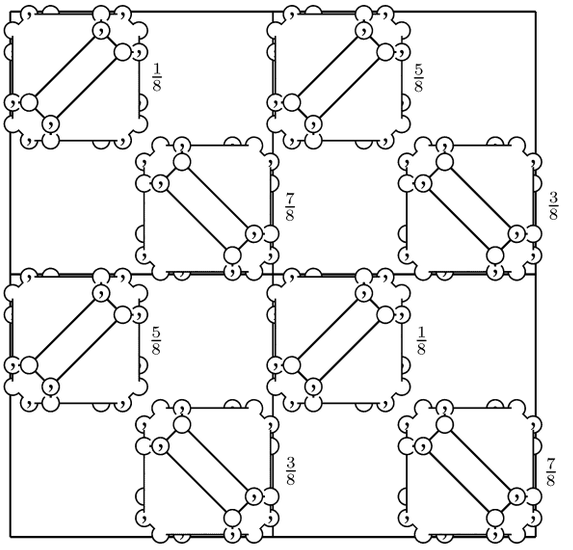
Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,\frac{1}{8}$

No. 227 $F\ 4_1/d\ \bar{3}\ 2/m$ Patterson symmetry $F\,m\,\bar{3}\,m$

ORIGIN CHOICE 2



Upper left quadrant only



Origin at centre $(\bar{3}\,m)$, at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ from $\bar{4}\,3\,m$

Asymmetric unit $-\frac{1}{8}\le x\le\frac{3}{8}$; $-\frac{1}{8}\le y\le 0$; $-\frac{1}{4}\le z\le 0$; $y\le\min(\frac{1}{4}-x,x)$; $-y-\frac{1}{4}\le z\le y$

Vertices $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{3}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{1}{4},0,0$ $0,0,0$ $\frac{1}{4},0,-\frac{1}{4}$ $0,0,-\frac{1}{4}$

Symmetry operations

For $(0,0,0)+$ set

(1) 1
(2) $2(0,0,\frac{1}{2})$ $\frac{3}{8},\frac{1}{8},z$
(3) $2(0,\frac{1}{2},0)$ $\frac{1}{8},y,\frac{3}{8}$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{3}{8},\frac{1}{8}$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x}+\frac{1}{2},x+\frac{1}{4},\bar{x}$
(7) 3^+ $x+\frac{3}{4},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$
(9) 3^- x,x,x
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{5}{12},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{7}{12},\bar{x}+\frac{5}{12},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{7}{12},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{4}$
(14) 2 $x,\bar{x},0$
(15) $4^-(0,0,\frac{3}{4})$ $\frac{3}{8},\frac{1}{8},z$
(16) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{8},\frac{5}{8},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{3}{8},\frac{1}{8}$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y+\frac{1}{4},y$
(19) 2 $0,y,\bar{y}$
(20) $4^+(\frac{1}{4},0,0)$ $x,-\frac{1}{8},\frac{5}{8}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{5}{8},y,-\frac{1}{8}$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{1}{4},x$
(23) $4^-(0,\frac{3}{4},0)$ $\frac{1}{8},y,\frac{3}{8}$
(24) 2 $\bar{x},0,x$
(25) $\bar{1}$ $0,0,0$
(26) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{1}{4}$
(27) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{1}{4},z$
(28) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{1}{4},y,z$
(29) $\bar{3}^+$ x,x,x; $0,0,0$
(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{3}{4},\bar{x}$; $-\frac{1}{4},0,\frac{3}{4}$
(31) $\bar{3}^+$ $x-\frac{1}{4},\bar{x}+1,\bar{x}$; $0,\frac{3}{4},-\frac{1}{4}$
(32) $\bar{3}^+$ $\bar{x}+\frac{3}{4},\bar{x}-\frac{1}{4},x$; $\frac{3}{4},-\frac{1}{4},0$
(33) $\bar{3}^-$ x,x,x; $0,0,0$
(34) $\bar{3}^-$ $x+\frac{5}{4},\bar{x}-1,\bar{x}$; $\frac{1}{2},-\frac{1}{4},\frac{3}{4}$
(35) $\bar{3}^-$ $\bar{x}+\frac{1}{4},\bar{x}+\frac{5}{4},x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{2}$
(36) $\bar{3}^-$ $\bar{x}+1,x+\frac{1}{4},\bar{x}$; $\frac{3}{4},\frac{1}{2},-\frac{1}{4}$
(37) $g(-\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{2},\bar{x},z$
(38) m x,x,z
(39) $\bar{4}^-$ $\frac{1}{8},\frac{5}{8},z$; $\frac{1}{8},\frac{5}{8},\frac{1}{8}$
(40) $\bar{4}^+$ $\frac{3}{8},-\frac{1}{8},z$; $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$
(41) $\bar{4}^-$ $x,\frac{1}{8},\frac{5}{8}$; $\frac{1}{8},\frac{1}{8},\frac{5}{8}$
(42) $g(\frac{1}{2},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$
(43) m x,y,y
(44) $\bar{4}^+$ $x,\frac{3}{8},-\frac{1}{8}$; $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$
(45) $\bar{4}^+$ $-\frac{1}{8},y,\frac{3}{8}$; $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$
(46) $g(\frac{1}{4},\frac{1}{2},-\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{5}{8},y,\frac{1}{8}$; $\frac{5}{8},\frac{1}{8},\frac{1}{8}$
(48) m x,y,x

For $(0,\frac{1}{2},\frac{1}{2})+$ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$
(2) 2 $\frac{3}{8},\frac{3}{8},z$
(3) 2 $\frac{1}{8},y,\frac{1}{8}$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{8},\frac{3}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{5}{12},\bar{x}$
(7) 3^+ $x+\frac{3}{4},\bar{x},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$
(10) 3^- $x+\frac{1}{4},\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x$
(12) 3^- $\bar{x},x+\frac{3}{4},\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)$ $x,x,0$
(14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{4})$ $\frac{1}{8},-\frac{1}{8},z$
(16) $4^+(0,0,\frac{3}{4})$ $\frac{1}{8},\frac{3}{8},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{3}{8},-\frac{3}{8}$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y-\frac{1}{4},y$
(19) 2 $0,y+\frac{1}{2},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)$ $x,-\frac{1}{8},\frac{1}{8}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{3}{8},y,-\frac{3}{8}$
(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x,0,x$
(23) $4^-(0,\frac{1}{4},0)$ $-\frac{1}{8},y,\frac{5}{8}$
(24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$
(26) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,0$
(27) $d(\frac{3}{4},0,\frac{3}{4})$ $x,0,z$
(28) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{1}{4},y,z$
(29) $\bar{3}^+$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$
(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{5}{4},\bar{x}$; $-\frac{1}{4},\frac{1}{2},\frac{3}{4}$
(31) $\bar{3}^+$ $x-\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$; $0,\frac{1}{4},-\frac{1}{4}$
(32) $\bar{3}^+$ $\bar{x}+\frac{3}{4},\bar{x}-\frac{3}{4},x$; $\frac{3}{4},-\frac{3}{4},0$
(33) $\bar{3}^-$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$
(34) $\bar{3}^-$ $x+\frac{3}{4},\bar{x}-\frac{3}{2},\bar{x}$; $0,-\frac{3}{4},\frac{3}{4}$
(35) $\bar{3}^-$ $\bar{x}-\frac{1}{4},\bar{x}+\frac{3}{4},x$; $-\frac{1}{4},\frac{3}{4},0$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x-\frac{1}{4},\bar{x}$; $\frac{1}{4},0,-\frac{1}{4}$
(37) m $x+\frac{1}{4},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x-\frac{1}{4},x,z$
(39) $\bar{4}^-$ $\frac{3}{8},\frac{3}{8},z$; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(40) $\bar{4}^+$ $\frac{5}{8},\frac{1}{8},z$; $\frac{5}{8},\frac{1}{8},\frac{1}{8}$
(41) $\bar{4}^-$ $x,\frac{1}{8},\frac{1}{8}$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$
(42) $g(\frac{1}{2},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$
(43) $g(0,\frac{1}{2},\frac{1}{2})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{3}{8},\frac{3}{8}$; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(45) $\bar{4}^+$ $\frac{1}{8},y,\frac{1}{8}$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$
(46) m $\bar{x}+\frac{3}{4},y,x$
(47) $\bar{4}^-$ $\frac{3}{8},y,-\frac{1}{8}$; $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$
(48) $g(\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $x-\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})+$ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$
(2) 2 $\frac{1}{8},\frac{1}{8},z$
(3) $2(0,\frac{1}{2},0)$ $\frac{3}{8},y,\frac{1}{8}$
(4) 2 $x,\frac{3}{8},\frac{3}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$
(6) 3^+ $\bar{x},x+\frac{3}{4},\bar{x}$
(7) 3^+ $x+\frac{1}{4},\bar{x},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{5}{12},\bar{x}+\frac{7}{12},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$
(10) 3^- $x+\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$
(11) 3^- $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$
(12) 3^- $\bar{x},x+\frac{1}{4},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x,0$
(14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},\frac{1}{4}$
(15) $4^-(0,0,\frac{1}{4})$ $\frac{5}{8},-\frac{1}{8},z$
(16) $4^+(0,0,\frac{3}{4})$ $-\frac{3}{8},\frac{3}{8},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{1}{8},-\frac{1}{8}$
(18) $2(0,\frac{3}{4},\frac{3}{4})$ $0,y,y$
(19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)$ $x,\frac{1}{8},\frac{3}{8}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{8},y,-\frac{1}{8}$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{1}{4},x$
(23) $4^-(0,\frac{3}{4},0)$ $-\frac{3}{8},y,\frac{3}{8}$
(24) 2 $\bar{x}+\frac{1}{2},0,x$
(25) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$
(26) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,0$
(27) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{1}{4},z$
(28) $d(0,\frac{1}{4},\frac{1}{4})$ $0,y,z$
(29) $\bar{3}^+$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{4},\bar{x}$; $-\frac{1}{4},0,\frac{1}{4}$
(31) $\bar{3}^+$ $x-\frac{3}{4},\bar{x}+\frac{3}{2},\bar{x}$; $0,\frac{3}{4},-\frac{3}{4}$
(32) $\bar{3}^+$ $\bar{x}+\frac{5}{4},\bar{x}+\frac{1}{4},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{2}$
(33) $\bar{3}^-$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$
(34) $\bar{3}^-$ $x+\frac{3}{4},\bar{x}-1,\bar{x}$; $0,-\frac{1}{4},\frac{3}{4}$
(35) $\bar{3}^-$ $\bar{x}-\frac{1}{4},\bar{x}+\frac{1}{4},x$; $-\frac{1}{4},\frac{1}{4},0$
(36) $\bar{3}^-$ $\bar{x}+\frac{3}{2},x-\frac{3}{4},\bar{x}$; $\frac{3}{4},0,-\frac{3}{4}$
(37) m $x+\frac{3}{4},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{4},x,z$
(39) $\bar{4}^-$ $-\frac{1}{8},\frac{3}{8},z$; $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$
(40) $\bar{4}^+$ $\frac{1}{8},\frac{1}{8},z$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$
(41) $\bar{4}^-$ $x,\frac{3}{8},\frac{3}{8}$; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(42) m $x,y+\frac{1}{4},\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{5}{8},\frac{1}{8}$; $\frac{1}{8},\frac{5}{8},\frac{1}{8}$
(45) $\bar{4}^+$ $\frac{3}{8},y,\frac{3}{8}$; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(46) $g(-\frac{1}{4},\frac{1}{2},\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{1}{8},y,\frac{1}{8}$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$
(48) $g(\frac{1}{2},0,\frac{1}{2})$ x,y,x

For $(\frac{1}{2},\frac{1}{2},0)+$ set

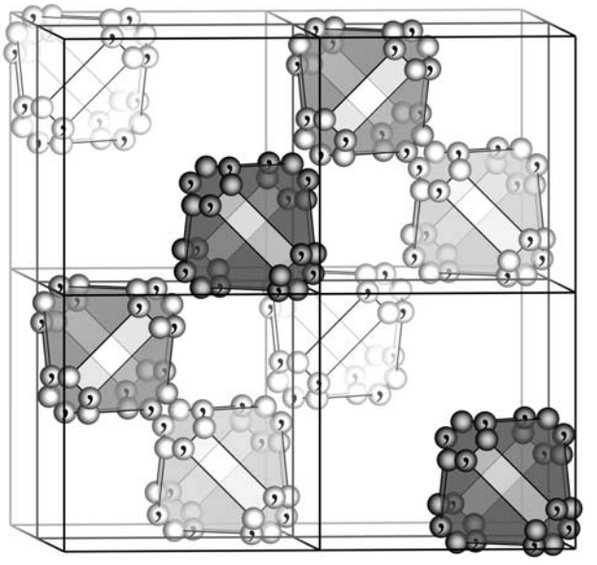
(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{8},\frac{3}{8},z$
(3) 2 $\frac{3}{8},y,\frac{3}{8}$
(4) 2 $x,\frac{1}{8},\frac{1}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$
(6) 3^+ $\bar{x},x+\frac{1}{4},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{7}{12},\bar{x}-\frac{1}{6},\bar{x}$
(8) 3^+ $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$
(10) 3^- $x+\frac{3}{4},\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$
(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{3}{4},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{1}{4}$
(14) 2 $x,\bar{x}+\frac{1}{2},0$
(15) $4^-(0,0,\frac{3}{4})$ $\frac{3}{8},-\frac{3}{8},z$
(16) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{8},\frac{1}{8},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{5}{8},-\frac{1}{8}$
(18) $2(0,\frac{1}{4},\frac{1}{4})$ $0,y,y$
(19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{1}{4},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)$ $x,-\frac{3}{8},\frac{3}{8}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{3}{8},y,\frac{1}{8}$
(22) $2(\frac{3}{4},0,\frac{3}{4})$ $x,0,x$
(23) $4^-(0,\frac{1}{4},0)$ $-\frac{1}{8},y,\frac{1}{8}$
(24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},\frac{1}{4},x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$
(26) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{1}{4}$
(27) $d(\frac{1}{4},0,\frac{1}{4})$ $x,0,z$
(28) $d(0,\frac{3}{4},\frac{3}{4})$ $0,y,z$
(29) $\bar{3}^+$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$
(30) $\bar{3}^+$ $\bar{x}-\frac{3}{2},x+\frac{3}{4},\bar{x}$; $-\frac{3}{4},0,\frac{3}{4}$
(31) $\bar{3}^+$ $x+\frac{1}{4},\bar{x}+1,\bar{x}$; $\frac{1}{2},\frac{3}{4},-\frac{1}{4}$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{4},\bar{x}-\frac{1}{4},x$; $\frac{1}{4},-\frac{1}{4},0$
(33) $\bar{3}^-$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$
(34) $\bar{3}^-$ $x+\frac{1}{4},\bar{x}-\frac{1}{2},\bar{x}$; $0,-\frac{1}{4},\frac{1}{4}$
(35) $\bar{3}^-$ $\bar{x}-\frac{3}{4},\bar{x}+\frac{3}{4},x$; $-\frac{3}{4},\frac{3}{4},0$
(36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{4},\bar{x}$; $\frac{3}{4},0,-\frac{1}{4}$
(37) $g(\frac{1}{4},-\frac{1}{4},\frac{1}{2})$ $x+\frac{1}{2},\bar{x},z$
(38) $g(\frac{1}{2},\frac{1}{2},0)$ x,x,z
(39) $\bar{4}^-$ $\frac{1}{8},\frac{1}{8},z$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$
(40) $\bar{4}^+$ $\frac{3}{8},\frac{3}{8},z$; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(41) $\bar{4}^-$ $x,-\frac{1}{8},\frac{3}{8}$; $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$
(42) m $x,y+\frac{3}{4},\bar{y}$
(43) $g(\frac{1}{2},\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{1}{8},\frac{1}{8}$; $\frac{1}{8},\frac{1}{8},\frac{1}{8}$
(45) $\bar{4}^+$ $\frac{1}{8},y,\frac{5}{8}$; $\frac{1}{8},\frac{1}{8},\frac{5}{8}$
(46) m $\bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-$ $\frac{3}{8},y,\frac{3}{8}$; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(48) $g(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{4},y,x$

ORIGIN CHOICE 2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							h,k,l permutable
							General:
192	i	1	(1) x,y,z	(2) $\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{4},y+\frac{1}{2},\bar{z}+\frac{3}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4}$	hkl: $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{y}+\frac{1}{4}$	(7) $\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{y}+\frac{3}{4}$	
			(9) y,z,x	(10) $\bar{y}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	(12) $\bar{y}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$	$0kl$: $k+l=4n$ and $k,l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$	
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{2}$	(18) $\bar{x}+\frac{1}{2},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{2},y+\frac{3}{4}$	hhl: $h+l=2n$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{2}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{2},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{2},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z},\bar{y},\bar{x}$	$h00$: $h=4n$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{3}{4},\bar{y}+\frac{1}{2},z+\frac{1}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{4},z+\frac{3}{4}$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{3}{4},\bar{x}+\frac{1}{2},y+\frac{1}{4}$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{3}{4},\bar{z}+\frac{1}{2},x+\frac{1}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{1}{2}$	
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y}+\frac{3}{4},x+\frac{1}{2},\bar{z}+\frac{1}{4}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) x,z,y	(44) $\bar{x}+\frac{3}{4},z+\frac{1}{2},\bar{y}+\frac{1}{4}$	
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{1}{2}$	(46) $\bar{z}+\frac{3}{4},y+\frac{1}{2},\bar{x}+\frac{1}{4}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) z,y,x	
							Special: as above, plus
96	h	. . 2	$0,y,\bar{y}$	$\frac{3}{4},\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2}$	$\frac{1}{4},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{1}{2},\bar{y}+\frac{3}{4},y+\frac{1}{4}$	no extra conditions
			$\bar{y},0,y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}+\frac{1}{4}$	$y+\frac{3}{4},\frac{1}{4},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{1}{2},\bar{y}+\frac{3}{4}$	
			$y,\bar{y},0$	$\bar{y}+\frac{1}{4},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{1}{4}$	$\bar{y}+\frac{3}{4},y+\frac{1}{4},\frac{1}{2}$	
			$0,\bar{y},y$	$\frac{1}{4},y+\frac{3}{4},y+\frac{1}{2}$	$\frac{3}{4},\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4}$	$\frac{1}{2},y+\frac{1}{4},\bar{y}+\frac{3}{4}$	
			$y,0,\bar{y}$	$y+\frac{1}{2},\frac{1}{4},y+\frac{3}{4}$	$\bar{y}+\frac{1}{4},\frac{3}{4},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{3}{4},\frac{1}{2},y+\frac{1}{4}$	
			$\bar{y},y,0$	$y+\frac{3}{4},y+\frac{1}{2},\frac{1}{4}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{4}$	$y+\frac{1}{4},\bar{y}+\frac{3}{4},\frac{1}{2}$	
96	g	. . m	x,x,z	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},z+\frac{1}{2}$	$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{z}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4}$	no extra conditions
			z,x,x	$z+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$	$\bar{z}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$	
			x,z,x	$\bar{x}+\frac{1}{4},z+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{z}+\frac{3}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{z}+\frac{1}{4},x+\frac{1}{2}$	
			$x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{z}$	$x+\frac{1}{4},\bar{x}+\frac{1}{2},z+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},z+\frac{1}{4}$	
			$x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$	$\bar{x},\bar{z},\bar{x}$	$x+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$	
			$z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$z+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{z}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$	$\bar{z},\bar{x},\bar{x}$	
48	f	2 . mm	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{3}{4},\frac{1}{8},\frac{5}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{5}{8},\bar{x}+\frac{3}{4},\frac{1}{8}$	$\frac{1}{8},\frac{1}{8},x$	$\frac{1}{8},\frac{5}{8},\bar{x}+\frac{3}{4}$	hkl: $h=2n+1$ or $h+k+l=4n$
			$\frac{7}{8},x+\frac{1}{4},\frac{3}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{3}{8}$	$\bar{x}+\frac{1}{2},\frac{7}{8},\frac{3}{8}$	$\frac{7}{8},\frac{3}{8},\bar{x}+\frac{1}{2}$	$\frac{3}{8},\frac{3}{8},x+\frac{3}{4}$	
32	e	. 3 m	x,x,x	$\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x+\frac{1}{2}$					no extra conditions
			$\bar{x}+\frac{1}{4},x+\frac{1}{2},\bar{x}+\frac{3}{4}$	$x+\frac{1}{2},\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4}$					
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{x},\bar{x}$					
			$x+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$					
16	d	. $\bar{3}$ m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$			hkl: $h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16	c	. $\bar{3}$ m	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$			
8	b	$\bar{4}$ 3 m	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$\frac{1}{8},\frac{5}{8},\frac{1}{8}$					hkl: $h=2n+1$ or $h+k+l=4n$
8	a	$\bar{4}$ 3 m	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{3}{8}$					



Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{8},\frac{3}{8},z$

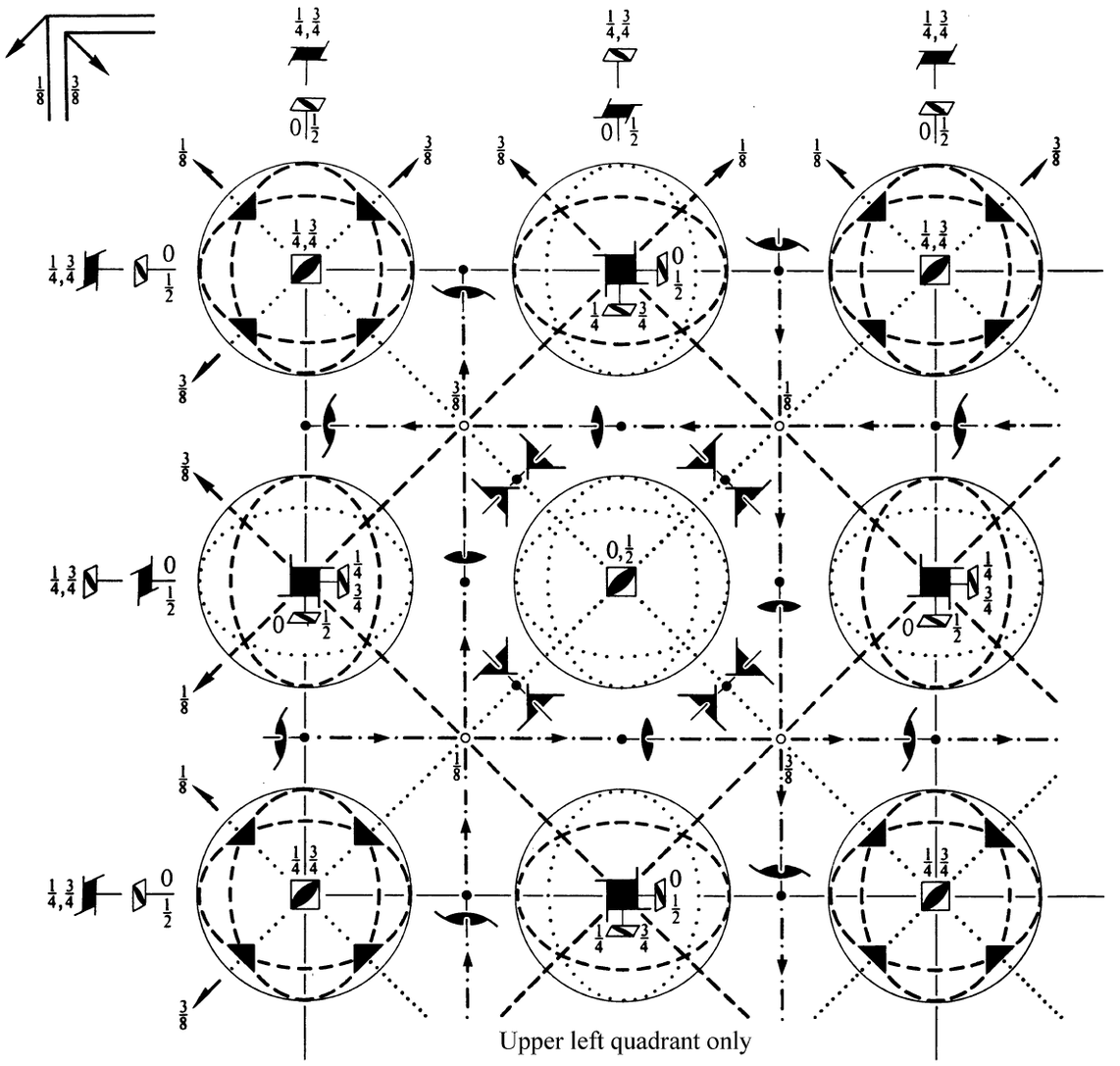
Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,x,0$

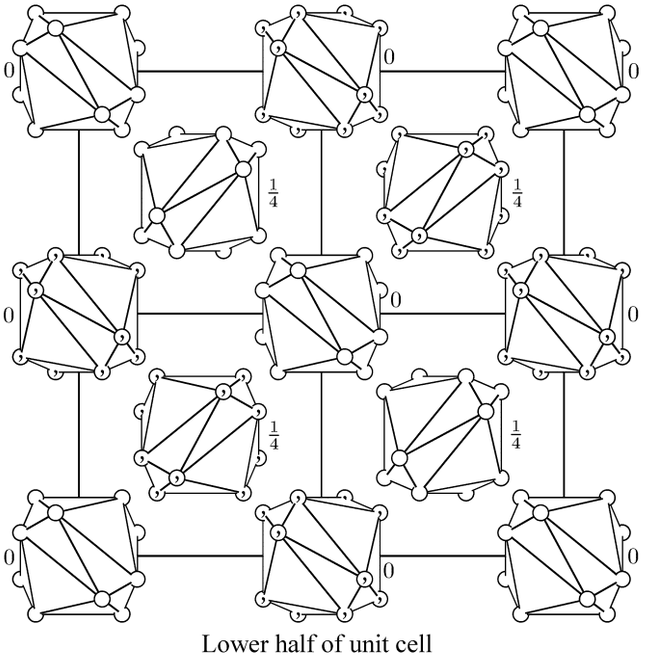
$F\,d\,\bar{3}\,c$ O_h^8 $m\bar{3}m$ Cubic

No. 228 $F\ 4_1/d\ \bar{3}\ 2/c$ Patterson symmetry $F\,m\bar{3}m$

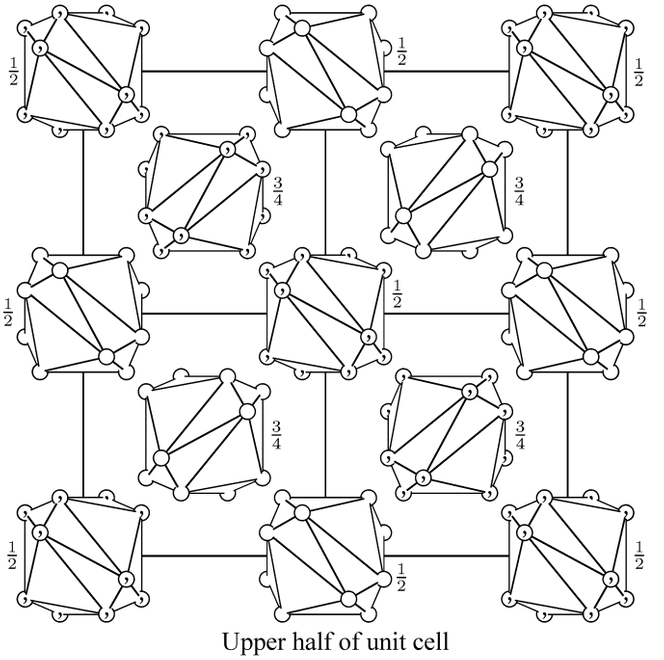
ORIGIN CHOICE 1



Upper left quadrant only



Lower half of unit cell



Upper half of unit cell

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Origin at 2 3, at $-\frac{3}{8},-\frac{3}{8},-\frac{3}{8}$ from centre $(\bar{3})$

Asymmetric unit $0\le x\le\frac{1}{2}$; $0\le y\le\frac{1}{8}$; $-\frac{1}{8}\le z\le\frac{1}{8}$; $y\le\min(\frac{1}{2}-x,x)$; $-y\le z\le y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{3}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},-\frac{1}{8}$

Symmetry operations

For (0,0,0)+ set

(1) 1
(2) $2(0,0,\frac{1}{2})$ $0,\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,0$
(4) $2(\frac{1}{2},0,0)$ $x,0,\frac{1}{4}$
(5) 3^+ x,x,x
(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{1}{6},\bar{x}$
(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},\bar{x}-\frac{1}{6},\bar{x}$
(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{6},\bar{x}+\frac{1}{3},x$
(9) 3^- x,x,x
(10) 3^- $x,\bar{x}+\frac{1}{2},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x},x$
(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{3}{8}$
(14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{4})$ $0,\frac{3}{4},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y+\frac{1}{4},y$
(19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{3}{4}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{3}{4},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{3}{8},x$
(23) $4^-(0,\frac{3}{4},0)$ $\frac{1}{4},y,\frac{1}{2}$
(24) 2 $\bar{x}+\frac{1}{4},\frac{1}{8},x$
(25) $\bar{1}$ $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(26) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{1}{8}$
(27) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{1}{8},z$
(28) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{1}{8},y,z$
(29) $\bar{3}^+$ x,x,x; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(30) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{3}{8},\frac{3}{8},\frac{5}{8}$
(31) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}$; $\frac{3}{8},\frac{5}{8},-\frac{3}{8}$
(32) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{5}{8},-\frac{3}{8},\frac{3}{8}$
(33) $\bar{3}^-$ x,x,x; $\frac{3}{8},\frac{3}{8},\frac{3}{8}$
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-1,\bar{x}$; $-\frac{1}{8},-\frac{3}{8},\frac{5}{8}$
(35) $\bar{3}^-$ $\bar{x}-\frac{1}{2},\bar{x}+\frac{1}{2},x$; $-\frac{3}{8},\frac{5}{8},-\frac{1}{8}$
(36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{2},\bar{x}$; $\frac{5}{8},-\frac{1}{8},-\frac{3}{8}$
(37) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$
(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z
(39) $\bar{4}^-$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$
(40) $\bar{4}^+$ $0,0,z$; $0,0,\frac{1}{4}$
(41) $\bar{4}^-$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$
(42) $g(0,-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y
(44) $\bar{4}^+$ $x,0,0$; $\frac{1}{4},0,0$
(45) $\bar{4}^+$ $0,y,0$; $0,\frac{1}{4},0$
(46) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$
(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

For $(0,\frac{1}{2},\frac{1}{2})$+ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$
(2) 2 $0,0,z$
(3) 2 $\frac{1}{4},y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$
(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$
(7) 3^+ $x,\bar{x},\bar{x}$
(8) 3^+ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$
(10) 3^- $x+\frac{1}{2},\bar{x},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) 3^- $\bar{x},x,\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)$ $x,x,\frac{1}{8}$
(14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$
(15) $4^-(0,0,\frac{1}{4})$ $\frac{1}{4},0,z$
(16) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{2},-\frac{1}{4}$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y-\frac{1}{4},y$
(19) 2 $\frac{1}{8},y+\frac{3}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)$ $x,0,\frac{1}{4}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,-\frac{1}{4}$
(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{8},x$
(23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{3}{4}$
(24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}$ $\frac{3}{8},\frac{1}{8},\frac{1}{8}$
(26) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,\frac{3}{8}$
(27) $d(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{3}{8},z$
(28) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{1}{8},y,z$
(29) $\bar{3}^+$ $x,x-\frac{1}{2},x$; $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$
(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{1}{2},\bar{x}$; $-\frac{3}{8},-\frac{1}{8},\frac{5}{8}$
(31) $\bar{3}^+$ $x,\bar{x}+\frac{3}{2},\bar{x}$; $\frac{3}{8},\frac{9}{8},-\frac{3}{8}$
(32) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{5}{8},\frac{1}{8},\frac{3}{8}$
(33) $\bar{3}^-$ $x+\frac{1}{2},x+\frac{1}{2},x$; $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$
(34) $\bar{3}^-$ $x+1,\bar{x}-\frac{1}{2},\bar{x}$; $\frac{3}{8},\frac{1}{8},\frac{5}{8}$
(35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{3}{8},\frac{5}{8},\frac{3}{8}$
(36) $\bar{3}^-$ $\bar{x}+\frac{3}{2},x,\bar{x}$; $\frac{9}{8},\frac{3}{8},-\frac{3}{8}$
(37) c $x,\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$
(39) $\bar{4}^-$ $0,\frac{1}{2},z$; $0,\frac{1}{2},\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{4},\frac{1}{4},z$; $\frac{1}{4},\frac{1}{4},0$
(41) $\bar{4}^-$ $x,-\frac{1}{4},\frac{1}{4}$; $0,-\frac{1}{4},\frac{1}{4}$
(42) $g(0,\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{4},\bar{y}$
(43) a x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{2},0$; $\frac{1}{4},\frac{1}{2},0$
(45) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{4}$; $-\frac{1}{4},0,\frac{1}{4}$
(46) b $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $0,y,0$; $0,\frac{1}{4},0$
(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})$+ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$
(2) 2 $\frac{1}{4},\frac{1}{4},z$
(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$
(4) 2 $x,0,0$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$
(6) 3^+ $\bar{x},x,\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x},\bar{x}$
(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) 3^- $\bar{x},\bar{x},x$
(12) 3^- $\bar{x},x+\frac{1}{2},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x,\frac{1}{8}$
(14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{2},\frac{3}{8}$
(15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(16) $4^+(0,0,\frac{3}{4})$ $-\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{1}{4},0$
(18) $2(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{8},y,y$
(19) $2(0,-\frac{1}{4},\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)$ $x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{4},y,0$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{3}{8},x$
(23) $4^-(0,\frac{3}{4},0)$ $-\frac{1}{4},y,\frac{1}{2}$
(24) 2 $\bar{x}+\frac{3}{4},\frac{1}{8},x$
(25) $\bar{1}$ $\frac{1}{8},\frac{3}{8},\frac{1}{8}$
(26) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,\frac{3}{8}$
(27) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{1}{8},z$
(28) $d(0,\frac{3}{4},\frac{3}{4})$ $\frac{3}{8},y,z$
(29) $\bar{3}^+$ $x+\frac{1}{2},x+\frac{1}{2},x$; $\frac{3}{8},\frac{3}{8},-\frac{1}{8}$
(30) $\bar{3}^+$ $\bar{x}-\frac{3}{2},x+\frac{3}{2},\bar{x}$; $-\frac{3}{8},\frac{3}{8},\frac{9}{8}$
(31) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{3}{8},\frac{5}{8},\frac{1}{8}$
(32) $\bar{3}^+$ $\bar{x}+\frac{1}{2},\bar{x}-\frac{1}{2},x$; $\frac{5}{8},-\frac{3}{8},-\frac{1}{8}$
(33) $\bar{3}^-$ $x-\frac{1}{2},x,x$; $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$
(34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}$; $\frac{3}{8},-\frac{3}{8},\frac{5}{8}$
(35) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{3}{2},x$; $-\frac{3}{8},\frac{9}{8},\frac{3}{8}$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$; $\frac{5}{8},\frac{3}{8},\frac{1}{8}$
(37) c $x+\frac{1}{2},\bar{x},z$
(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$
(39) $\bar{4}^-$ $0,0,z$; $0,0,\frac{1}{4}$
(40) $\bar{4}^+$ $\frac{1}{4},-\frac{1}{4},z$; $\frac{1}{4},-\frac{1}{4},0$
(41) $\bar{4}^-$ $x,0,\frac{1}{2}$; $\frac{1}{4},0,\frac{1}{2}$
(42) a $x,y,\bar{y}$
(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{1}{4},\frac{1}{4}$; $0,\frac{1}{4},\frac{1}{4}$
(45) $\bar{4}^+$ $0,y,\frac{1}{2}$; $0,\frac{1}{4},\frac{1}{2}$
(46) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,-\frac{1}{4}$; $\frac{1}{4},0,-\frac{1}{4}$
(48) b x,y,x

For $(\frac{1}{2},\frac{1}{2},0)$+ set

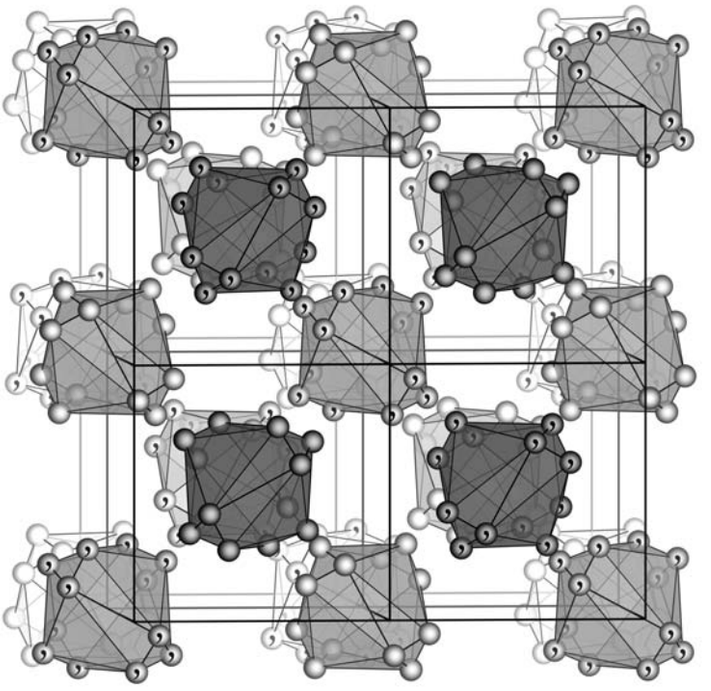
(1) $t(\frac{1}{2},\frac{1}{2},0)$
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(3) 2 $0,y,0$
(4) 2 $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$
(6) 3^+ $\bar{x},x+\frac{1}{2},\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x},\bar{x},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$
(10) 3^- $x,\bar{x},\bar{x}$
(11) 3^- $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$
(14) 2 $x,\bar{x}+\frac{3}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},-\frac{1}{4},z$
(16) $4^+(0,0,\frac{1}{4})$ $0,\frac{1}{4},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{4},0$
(18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{8},y,y$
(19) $2(0,\frac{1}{4},-\frac{1}{4})$ $\frac{3}{8},y+\frac{1}{2},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,\frac{1}{4}$
(22) $2(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{8},x$
(23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$
(24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{2},\frac{3}{8},x$
(25) $\bar{1}$ $\frac{1}{8},\frac{1}{8},\frac{3}{8}$
(26) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{1}{8}$
(27) $d(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{3}{8},z$
(28) $d(0,\frac{1}{4},\frac{1}{4})$ $\frac{3}{8},y,z$
(29) $\bar{3}^+$ $x-\frac{1}{2},x,x$; $-\frac{1}{8},\frac{3}{8},\frac{3}{8}$
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; $\frac{1}{8},\frac{3}{8},\frac{5}{8}$
(31) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+1,\bar{x}$; $-\frac{1}{8},\frac{5}{8},-\frac{3}{8}$
(32) $\bar{3}^+$ $\bar{x}+\frac{3}{2},\bar{x},x$; $\frac{9}{8},-\frac{3}{8},\frac{3}{8}$
(33) $\bar{3}^-$ $x,x-\frac{1}{2},x$; $\frac{3}{8},-\frac{1}{8},\frac{3}{8}$
(34) $\bar{3}^-$ $x+\frac{3}{2},\bar{x}-\frac{3}{2},\bar{x}$; $\frac{3}{8},-\frac{3}{8},\frac{9}{8}$
(35) $\bar{3}^-$ $\bar{x}+\frac{1}{2},\bar{x}+1,x$; $\frac{1}{8},\frac{5}{8},\frac{3}{8}$
(36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{5}{8},\frac{3}{8},-\frac{3}{8}$
(37) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{4},\bar{x},z$
(38) c x,x,z
(39) $\bar{4}^-$ $-\frac{1}{4},\frac{1}{4},z$; $-\frac{1}{4},\frac{1}{4},0$
(40) $\bar{4}^+$ $\frac{1}{2},0,z$; $\frac{1}{2},0,\frac{1}{4}$
(41) $\bar{4}^-$ $x,0,0$; $\frac{1}{4},0,0$
(42) a $x,y+\frac{1}{2},\bar{y}$
(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$
(44) $\bar{4}^+$ $x,\frac{1}{4},-\frac{1}{4}$; $0,\frac{1}{4},-\frac{1}{4}$
(45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{4}$; $\frac{1}{4},0,\frac{1}{4}$
(46) b $\bar{x},y,x$
(47) $\bar{4}^-$ $\frac{1}{2},y,0$; $\frac{1}{2},\frac{1}{4},0$
(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$

ORIGIN CHOICE 1

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							h,k,l permutable
							General:
192	h	1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$	
			(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$	$0kl$: $k+l=4n$ and $k,l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$	hhl: $h,l=2n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	$h00$: $h=4n$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
			(25) $\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(26) $x+\frac{3}{4},y+\frac{1}{4},\bar{z}+\frac{1}{4}$	(27) $x+\frac{1}{4},\bar{y}+\frac{1}{4},z+\frac{3}{4}$	(28) $\bar{x}+\frac{1}{4},y+\frac{3}{4},z+\frac{1}{4}$	
			(29) $\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(30) $\bar{z}+\frac{1}{4},x+\frac{3}{4},y+\frac{1}{4}$	(31) $z+\frac{3}{4},x+\frac{1}{4},\bar{y}+\frac{1}{4}$	(32) $z+\frac{1}{4},\bar{x}+\frac{1}{4},y+\frac{3}{4}$	
			(33) $\bar{y}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{x}+\frac{3}{4}$	(34) $y+\frac{1}{4},\bar{z}+\frac{1}{4},x+\frac{3}{4}$	(35) $\bar{y}+\frac{1}{4},z+\frac{3}{4},x+\frac{1}{4}$	(36) $y+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{4}$	
			(37) $\bar{y},\bar{x}+\frac{1}{2},z$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{1}{2},x,\bar{z}$	(40) $y,\bar{x},\bar{z}+\frac{1}{2}$	
			(41) $\bar{x},\bar{z}+\frac{1}{2},y$	(42) $x,\bar{z},\bar{y}+\frac{1}{2}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{1}{2},z,\bar{y}$	
			(45) $\bar{z},\bar{y}+\frac{1}{2},x$	(46) $\bar{z}+\frac{1}{2},y,\bar{x}$	(47) $z,\bar{y},\bar{x}+\frac{1}{2}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	
							Special: as above, plus
96	g	. . 2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{7}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{5}{8},\bar{y},y+\frac{1}{4}$	no extra conditions
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{7}{8},\bar{y}+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{8},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{5}{8},\bar{y}$	
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{7}{8}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{3}{8}$	$\bar{y},y+\frac{1}{4},\frac{5}{8}$	
			$\frac{5}{8},\bar{y}+\frac{3}{4},y+\frac{1}{2}$	$\frac{7}{8},y+\frac{1}{4},y$	$\frac{3}{8},\bar{y}+\frac{1}{4},\bar{y}$	$\frac{1}{8},y+\frac{3}{4},\bar{y}+\frac{1}{2}$	
			$y+\frac{1}{2},\frac{5}{8},\bar{y}+\frac{3}{4}$	$y,\frac{7}{8},y+\frac{1}{4}$	$\bar{y},\frac{3}{8},\bar{y}+\frac{1}{4}$	$\bar{y}+\frac{1}{2},\frac{1}{8},y+\frac{3}{4}$	
			$\bar{y}+\frac{3}{4},y+\frac{1}{2},\frac{5}{8}$	$y+\frac{1}{4},y,\frac{7}{8}$	$\bar{y}+\frac{1}{4},\bar{y},\frac{3}{8}$	$y+\frac{3}{4},\bar{y}+\frac{1}{2},\frac{1}{8}$	
96	f	2 . .	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$0,x,0$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$0,0,x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	hkl: $h+k+l=4n$
			$\frac{3}{4},x+\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},x+\frac{3}{4}$	
			$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\bar{x}+\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},x+\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x+\frac{3}{4}$	
			$0,\bar{x}+\frac{1}{2},0$	$\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},0$	$x,0,\frac{1}{2}$	$0,\frac{1}{2},x$	$\frac{1}{2},0,\bar{x}$	
64	e	. 3 .	x,x,x	$\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$	hkl: $h=2n$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$	
			$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$	
			$\bar{x},\bar{x}+\frac{1}{2},x$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x,\bar{x}$	$x,\bar{x},\bar{x}+\frac{1}{2}$	
48	d	$\bar{4}$ . .	$\frac{1}{4},0,0$	$\frac{3}{4},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},\frac{1}{2}$	$0,0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},\frac{3}{4}$	hkl: $h+k+l=4n$
			$\frac{3}{4},\frac{1}{2},\frac{3}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},0$	
32	c	. $\bar{3}$.	$\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$\frac{5}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{1}{8}$	$\frac{1}{8},\frac{5}{8},\frac{3}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{3}{8},\frac{1}{8}$	$\frac{3}{8},\frac{1}{8},\frac{5}{8}$	hkl: $h,k,l=4n+2$ or $h,k,l=4n$
32	b	. 3 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{3}{8}$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{7}{8},\frac{3}{8},\frac{1}{8}$	$\frac{3}{8},\frac{1}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{3}{8}$	hkl: $h,k,l=4n+2$ or $h,k,l=4n$
16	a	2 3 .	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$0,\frac{1}{2},0$	hkl: $h+k+l=4n$



Symmetry of special projections

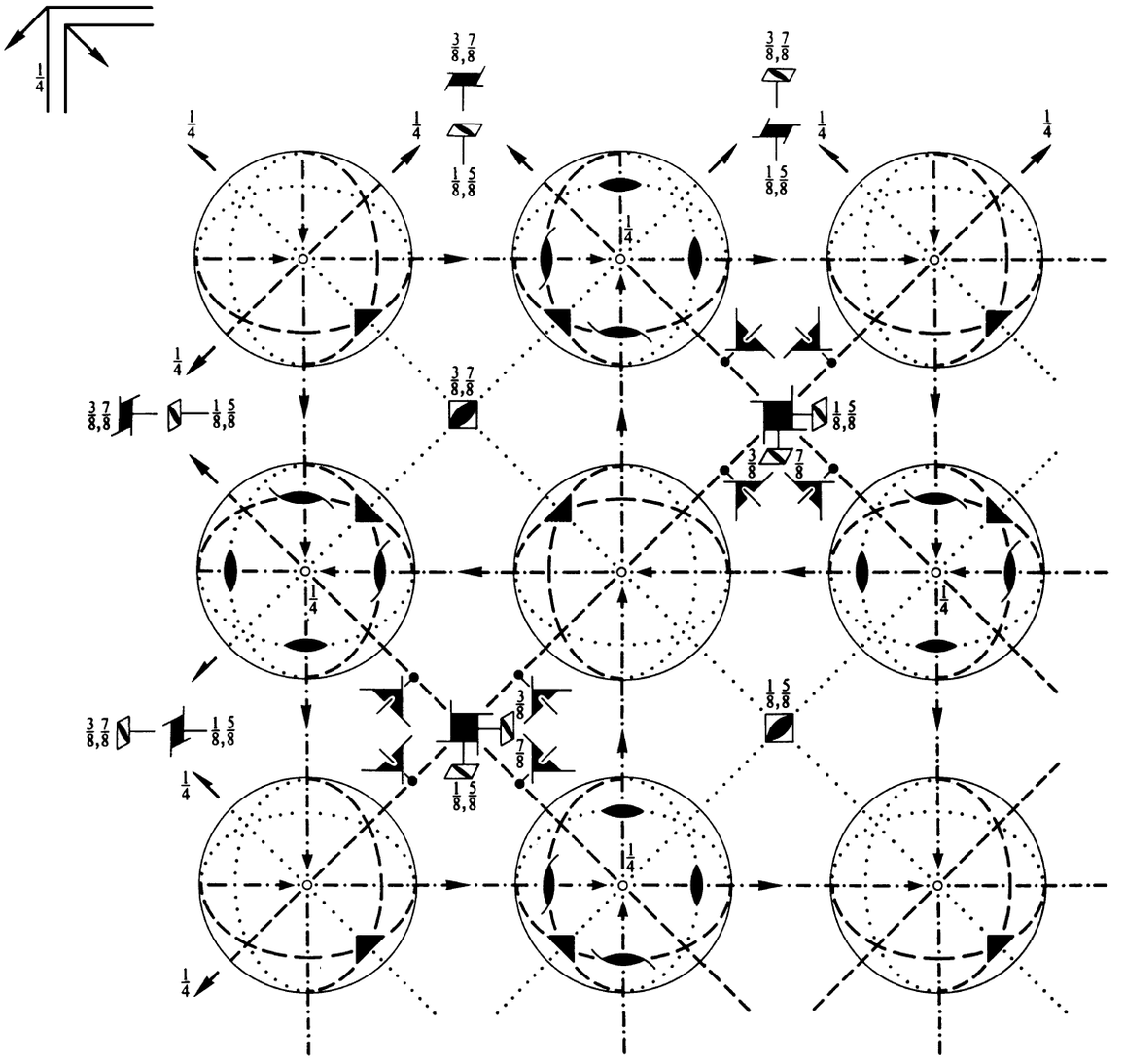
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

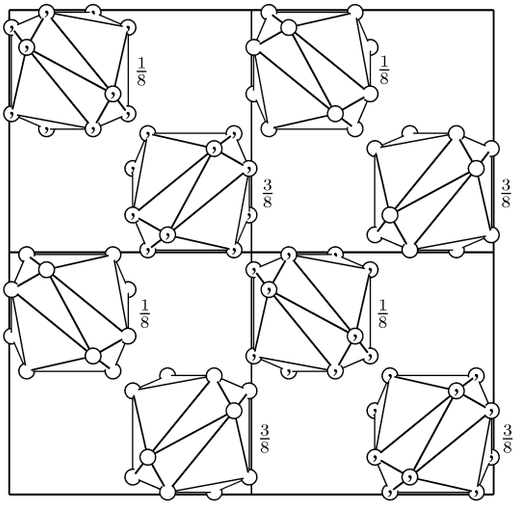
Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,\frac{1}{8}$

No. 228 $F\ 4_1/d\ \bar{3}\ 2/c$ Patterson symmetry $F\,m\,\bar{3}\,m$

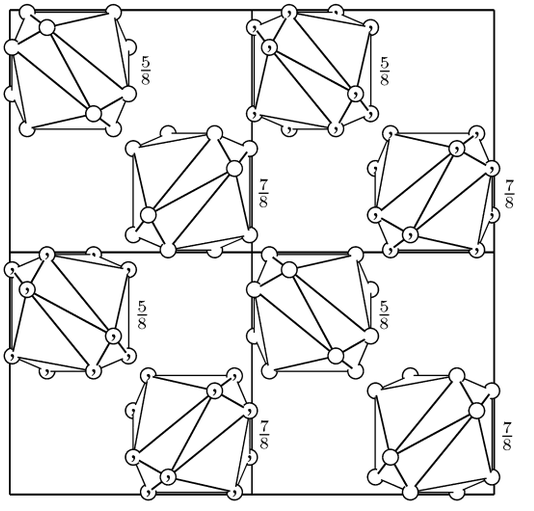
ORIGIN CHOICE 2



Upper left quadrant only



Lower half of unit cell



Upper half of unit cell

Origin at centre $(\bar{3})$, at $\frac{3}{8},\frac{3}{8},\frac{3}{8}$ from 2 3

Asymmetric unit $-\frac{1}{8}\le x\le\frac{3}{8}$; $-\frac{1}{8}\le y\le 0$; $-\frac{1}{4}\le z\le 0$; $y\le\min(\frac{1}{4}-x,x)$; $-y-\frac{1}{4}\le z\le y$

Vertices $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{3}{8},-\frac{1}{8},-\frac{1}{8}$ $\frac{1}{4},0,0$ $0,0,0$ $\frac{1}{4},0,-\frac{1}{4}$ $0,0,-\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{8},\frac{3}{8},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{3}{8},y,\frac{1}{8}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{8},\frac{3}{8}$
(5) 3^+ x,x,x	(6) $3^+(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}+\frac{1}{6},x+\frac{5}{12},\bar{x}$	(7) $3^+(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{7}{12},\bar{x}-\frac{1}{6},\bar{x}$	(8) $3^+(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{5}{12},\bar{x}+\frac{7}{12},x$
(9) 3^- x,x,x	(10) 3^- $x+\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$	(11) 3^- $\bar{x}+\frac{3}{4},\bar{x}+\frac{1}{4},x$	(12) 3^- $\bar{x}-\frac{1}{2},x+\frac{3}{4},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},0$	(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{8},-\frac{1}{8},z$	(16) $4^+(0,0,\frac{1}{4})$ $-\frac{3}{8},\frac{3}{8},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{8},-\frac{1}{8}$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $0,y+\frac{1}{4},y$	(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{4},0,0)$ $x,-\frac{3}{8},\frac{3}{8}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{3}{8},y,-\frac{3}{8}$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},0,x$	(23) $4^-(0,\frac{3}{4},0)$ $-\frac{1}{8},y,\frac{1}{8}$	(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}$ 0,0,0	(26) $d(\frac{3}{4},\frac{1}{4},0)$ $x,y,\frac{1}{4}$	(27) $d(\frac{1}{4},0,\frac{3}{4})$ $x,\frac{1}{4},z$	(28) $d(0,\frac{3}{4},\frac{1}{4})$ $\frac{1}{4},y,z$
(29) $\bar{3}^+$ x,x,x; 0,0,0	(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{5}{4},\bar{x}$; $-\frac{1}{4},\frac{1}{2},\frac{3}{4}$	(31) $\bar{3}^+$ $x+\frac{1}{4},\bar{x}+1,\bar{x}$; $\frac{1}{2},\frac{3}{4},-\frac{1}{4}$	(32) $\bar{3}^+$ $\bar{x}+\frac{5}{4},\bar{x}+\frac{1}{4},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{2}$
(33) $\bar{3}^-$ x,x,x; 0,0,0	(34) $\bar{3}^-$ $x+\frac{3}{4},\bar{x}-1,\bar{x}$; $0,-\frac{1}{4},\frac{3}{4}$	(35) $\bar{3}^-$ $\bar{x}-\frac{1}{4},\bar{x}+\frac{3}{4},x$; $-\frac{1}{4},\frac{3}{4},0$	(36) $\bar{3}^-$ $\bar{x}+1,x-\frac{1}{4},\bar{x}$; $\frac{3}{4},0,-\frac{1}{4}$
(37) $g(-\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{2},\bar{x},z$	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(39) $\bar{4}^-$ $\frac{3}{8},\frac{3}{8},z$; $\frac{3}{8},\frac{3}{8},\frac{1}{8}$	(40) $\bar{4}^+$ $\frac{1}{8},\frac{1}{8},z$; $\frac{1}{8},\frac{1}{8},\frac{3}{8}$
(41) $\bar{4}^-$ $x,\frac{3}{8},\frac{3}{8}$; $\frac{1}{8},\frac{3}{8},\frac{3}{8}$	(42) $g(0,-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(44) $\bar{4}^+$ $x,\frac{1}{8},\frac{1}{8}$; $\frac{3}{8},\frac{1}{8},\frac{1}{8}$
(45) $\bar{4}^+$ $\frac{1}{8},y,\frac{1}{8}$; $\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(46) $g(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^-$ $\frac{3}{8},y,\frac{3}{8}$; $\frac{3}{8},\frac{1}{8},\frac{3}{8}$	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

For $(0,\frac{1}{2},\frac{1}{2})$+ set

(1) $t(0,\frac{1}{2},\frac{1}{2})$	(2) 2 $\frac{1}{8},\frac{1}{8},z$	(3) 2 $\frac{3}{8},y,\frac{3}{8}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{3}{8},\frac{1}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{3},x-\frac{1}{6},x$	(6) 3^+ $\bar{x}+\frac{1}{2},x+\frac{1}{4},\bar{x}$	(7) 3^+ $x+\frac{1}{4},\bar{x},\bar{x}$	(8) 3^+ $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x+\frac{1}{6},x$	(10) 3^- $x+\frac{3}{4},\bar{x},\bar{x}$	(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{7}{12},\bar{x}+\frac{5}{12},x$	(12) 3^- $\bar{x},x+\frac{1}{4},\bar{x}$
(13) $2(\frac{3}{4},\frac{3}{4},0)$ $x,x,\frac{1}{4}$	(14) $2(\frac{1}{4},-\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},0$	(15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{8},\frac{1}{8},z$	(16) $4^+(0,0,\frac{3}{4})$ $-\frac{1}{8},\frac{1}{8},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{5}{8},-\frac{1}{8}$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $0,y-\frac{1}{4},y$	(19) 2 $\frac{1}{4},y,\bar{y}$	(20) $4^+(\frac{1}{4},0,0)$ $x,\frac{1}{8},\frac{3}{8}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{5}{8},y,-\frac{1}{8}$	(22) $2(\frac{1}{4},0,\frac{1}{4})$ $x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{4},0)$ $-\frac{3}{8},y,\frac{3}{8}$	(24) $2(\frac{1}{4},0,-\frac{1}{4})$ $\bar{x}+\frac{1}{4},0,x$
(25) $\bar{1}$ $0,\frac{1}{4},\frac{1}{4}$	(26) $d(\frac{3}{4},\frac{3}{4},0)$ $x,y,0$	(27) $d(\frac{1}{4},0,\frac{1}{4})$ $x,0,z$	(28) $d(0,\frac{1}{4},\frac{3}{4})$ $\frac{1}{4},y,z$
(29) $\bar{3}^+$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$	(30) $\bar{3}^+$ $\bar{x}-1,x+\frac{3}{4},\bar{x}$; $-\frac{1}{4},0,\frac{3}{4}$	(31) $\bar{3}^+$ $x-\frac{3}{4},\bar{x}+\frac{3}{2},\bar{x}$; $0,\frac{3}{4},-\frac{3}{4}$	(32) $\bar{3}^+$ $\bar{x}+\frac{1}{4},\bar{x}-\frac{1}{4},x$; $\frac{1}{4},-\frac{1}{4},0$
(33) $\bar{3}^-$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$	(34) $\bar{3}^-$ $x+\frac{1}{4},\bar{x}-\frac{1}{2},\bar{x}$; $0,-\frac{1}{4},\frac{1}{4}$	(35) $\bar{3}^-$ $\bar{x}+\frac{1}{4},\bar{x}+\frac{5}{4},x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{2}$	(36) $\bar{3}^-$ $\bar{x}+\frac{3}{2},x-\frac{3}{4},\bar{x}$; $\frac{3}{4},0,-\frac{3}{4}$
(37) c $x+\frac{1}{4},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x+\frac{1}{4},x,z$	(39) $\bar{4}^-$ $\frac{1}{8},\frac{5}{8},z$; $\frac{1}{8},\frac{5}{8},\frac{3}{8}$	(40) $\bar{4}^+$ $\frac{3}{8},\frac{3}{8},z$; $\frac{3}{8},\frac{3}{8},\frac{1}{8}$
(41) $\bar{4}^-$ $x,-\frac{1}{8},\frac{3}{8}$; $\frac{1}{8},-\frac{1}{8},\frac{3}{8}$	(42) $g(0,\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$	(43) a x,y,y	(44) $\bar{4}^+$ $x,\frac{5}{8},\frac{1}{8}$; $\frac{3}{8},\frac{5}{8},\frac{1}{8}$
(45) $\bar{4}^+$ $-\frac{1}{8},y,\frac{3}{8}$; $-\frac{1}{8},\frac{1}{8},\frac{3}{8}$	(46) b $\bar{x}+\frac{3}{4},y,x$	(47) $\bar{4}^-$ $\frac{1}{8},y,\frac{1}{8}$; $\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x+\frac{1}{4},y,x$

For $(\frac{1}{2},0,\frac{1}{2})$+ set

(1) $t(\frac{1}{2},0,\frac{1}{2})$	(2) 2 $\frac{3}{8},\frac{3}{8},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{8},y,\frac{3}{8}$	(4) 2 $x,\frac{1}{8},\frac{1}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x-\frac{1}{6},x$	(6) 3^+ $\bar{x},x+\frac{1}{4},\bar{x}$	(7) 3^+ $x+\frac{3}{4},\bar{x},\bar{x}$	(8) 3^+ $\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x-\frac{1}{6},x-\frac{1}{3},x$	(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{5}{12},\bar{x}+\frac{1}{6},\bar{x}$	(11) 3^- $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$	(12) 3^- $\bar{x},x+\frac{3}{4},\bar{x}$
(13) $2(\frac{1}{4},\frac{1}{4},0)$ $x,x,\frac{1}{4}$	(14) $2(-\frac{1}{4},\frac{1}{4},0)$ $x,\bar{x}+\frac{1}{4},0$	(15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{8},-\frac{3}{8},z$	(16) $4^+(0,0,\frac{3}{4})$ $-\frac{1}{8},\frac{5}{8},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{8},\frac{1}{8}$	(18) $2(0,\frac{3}{4},\frac{3}{4})$ $\frac{1}{4},y,y$	(19) $2(0,\frac{1}{4},-\frac{1}{4})$ $0,y+\frac{1}{4},\bar{y}$	(20) $4^+(\frac{3}{4},0,0)$ $x,-\frac{1}{8},\frac{1}{8}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{3}{8},y,\frac{1}{8}$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},0,x$	(23) $4^-(0,\frac{3}{4},0)$ $-\frac{1}{8},y,\frac{5}{8}$	(24) 2 $\bar{x},\frac{1}{4},x$
(25) $\bar{1}$ $\frac{1}{4},0,\frac{1}{4}$	(26) $d(\frac{1}{4},\frac{1}{4},0)$ $x,y,0$	(27) $d(\frac{3}{4},0,\frac{1}{4})$ $x,\frac{1}{4},z$	(28) $d(0,\frac{3}{4},\frac{3}{4})$ $0,y,z$
(29) $\bar{3}^+$ $x-\frac{1}{2},x-\frac{1}{2},x$; $0,0,\frac{1}{2}$	(30) $\bar{3}^+$ $\bar{x}-\frac{3}{2},x+\frac{3}{4},\bar{x}$; $-\frac{3}{4},0,\frac{3}{4}$	(31) $\bar{3}^+$ $x-\frac{1}{4},\bar{x}+\frac{1}{2},\bar{x}$; $0,\frac{1}{4},-\frac{1}{4}$	(32) $\bar{3}^+$ $\bar{x}+\frac{3}{4},\bar{x}-\frac{1}{4},x$; $\frac{3}{4},-\frac{1}{4},0$
(33) $\bar{3}^-$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$	(34) $\bar{3}^-$ $x+\frac{5}{4},\bar{x}-1,\bar{x}$; $\frac{1}{2},-\frac{1}{4},\frac{3}{4}$	(35) $\bar{3}^-$ $\bar{x}-\frac{3}{4},\bar{x}+\frac{3}{4},x$; $-\frac{3}{4},\frac{3}{4},0$	(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x-\frac{1}{4},\bar{x}$; $\frac{1}{4},0,-\frac{1}{4}$
(37) c $x+\frac{3}{4},\bar{x},z$	(38) $g(\frac{1}{4},\frac{1}{4},0)$ $x-\frac{1}{4},x,z$	(39) $\bar{4}^-$ $\frac{1}{8},\frac{1}{8},z$; $\frac{1}{8},\frac{1}{8},\frac{3}{8}$	(40) $\bar{4}^+$ $\frac{3}{8},-\frac{1}{8},z$; $\frac{3}{8},-\frac{1}{8},\frac{1}{8}$
(41) $\bar{4}^-$ $x,\frac{1}{8},\frac{5}{8}$; $\frac{3}{8},\frac{1}{8},\frac{5}{8}$	(42) a $x,y+\frac{1}{4},\bar{y}$	(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{4},y$	(44) $\bar{4}^+$ $x,\frac{3}{8},\frac{3}{8}$; $\frac{1}{8},\frac{3}{8},\frac{3}{8}$
(45) $\bar{4}^+$ $\frac{1}{8},y,\frac{5}{8}$; $\frac{1}{8},\frac{3}{8},\frac{5}{8}$	(46) $g(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^-$ $\frac{3}{8},y,-\frac{1}{8}$; $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$	(48) b x,y,x

For $(\frac{1}{2},\frac{1}{2},0)$+ set

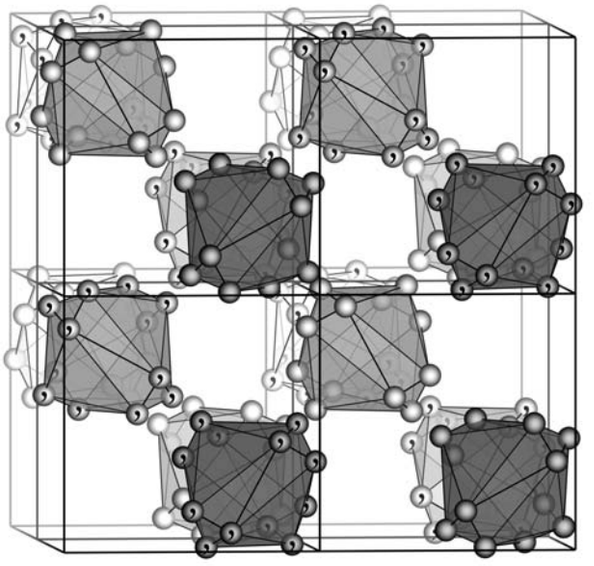
(1) $t(\frac{1}{2},\frac{1}{2},0)$	(2) $2(0,0,\frac{1}{2})$ $\frac{3}{8},\frac{1}{8},z$	(3) 2 $\frac{1}{8},y,\frac{1}{8}$	(4) 2 $x,\frac{3}{8},\frac{3}{8}$
(5) $3^+(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},x+\frac{1}{3},x$	(6) 3^+ $\bar{x},x+\frac{3}{4},\bar{x}$	(7) 3^+ $x+\frac{3}{4},\bar{x}-\frac{1}{2},\bar{x}$	(8) 3^+ $\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},x$
(9) $3^-(\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{3},x+\frac{1}{6},x$	(10) 3^- $x+\frac{1}{4},\bar{x},\bar{x}$	(11) 3^- $\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},x$	(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{7}{12},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},0$	(14) 2 $x,\bar{x},\frac{1}{4}$	(15) $4^-(0,0,\frac{3}{4})$ $\frac{5}{8},-\frac{1}{8},z$	(16) $4^+(0,0,\frac{1}{4})$ $\frac{1}{8},\frac{3}{8},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{8},-\frac{3}{8}$	(18) $2(0,\frac{1}{4},\frac{1}{4})$ $\frac{1}{4},y,y$	(19) $2(0,-\frac{1}{4},\frac{1}{4})$ $0,y+\frac{1}{4},\bar{y}$	(20) $4^+(\frac{3}{4},0,0)$ $x,-\frac{1}{8},\frac{5}{8}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{8},y,-\frac{1}{8}$	(22) $2(\frac{3}{4},0,\frac{3}{4})$ $x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{4},0)$ $\frac{1}{8},y,\frac{3}{8}$	(24) $2(-\frac{1}{4},0,\frac{1}{4})$ $\bar{x}+\frac{1}{4},0,x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},0$	(26) $d(\frac{1}{4},\frac{3}{4},0)$ $x,y,\frac{1}{4}$	(27) $d(\frac{3}{4},0,\frac{3}{4})$ $x,0,z$	(28) $d(0,\frac{1}{4},\frac{1}{4})$ $0,y,z$
(29) $\bar{3}^+$ $x+\frac{1}{2},x,x$; $\frac{1}{2},0,0$	(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+\frac{1}{4},\bar{x}$; $-\frac{1}{4},0,\frac{1}{4}$	(31) $\bar{3}^+$ $x-\frac{1}{4},\bar{x}+1,\bar{x}$; $0,\frac{3}{4},-\frac{1}{4}$	(32) $\bar{3}^+$ $\bar{x}+\frac{3}{4},\bar{x}-\frac{3}{4},x$; $\frac{3}{4},-\frac{3}{4},0$
(33) $\bar{3}^-$ $x,x+\frac{1}{2},x$; $0,\frac{1}{2},0$	(34) $\bar{3}^-$ $x+\frac{3}{4},\bar{x}-\frac{3}{2},\bar{x}$; $0,-\frac{3}{4},\frac{3}{4}$	(35) $\bar{3}^-$ $\bar{x}-\frac{1}{4},\bar{x}+\frac{1}{4},x$; $-\frac{1}{4},\frac{1}{4},0$	(36) $\bar{3}^-$ $\bar{x}+1,x+\frac{1}{4},\bar{x}$; $\frac{3}{4},\frac{1}{2},-\frac{1}{4}$
(37) $g(\frac{1}{4},-\frac{1}{4},0)$ $x+\frac{1}{2},\bar{x},z$	(38) c x,x,z	(39) $\bar{4}^-$ $-\frac{1}{8},\frac{3}{8},z$; $-\frac{1}{8},\frac{3}{8},\frac{1}{8}$	(40) $\bar{4}^+$ $\frac{5}{8},\frac{1}{8},z$; $\frac{5}{8},\frac{1}{8},\frac{3}{8}$
(41) $\bar{4}^-$ $x,\frac{1}{8},\frac{1}{8}$; $\frac{3}{8},\frac{1}{8},\frac{1}{8}$	(42) a $x,y+\frac{3}{4},\bar{y}$	(43) $g(0,\frac{1}{4},\frac{1}{4})$ $x,y-\frac{1}{4},y$	(44) $\bar{4}^+$ $x,\frac{3}{8},-\frac{1}{8}$; $\frac{1}{8},\frac{3}{8},-\frac{1}{8}$
(45) $\bar{4}^+$ $\frac{3}{8},y,\frac{3}{8}$; $\frac{3}{8},\frac{1}{8},\frac{3}{8}$	(46) b $\bar{x}+\frac{1}{4},y,x$	(47) $\bar{4}^-$ $\frac{5}{8},y,\frac{1}{8}$; $\frac{5}{8},\frac{3}{8},\frac{1}{8}$	(48) $g(\frac{1}{4},0,\frac{1}{4})$ $x-\frac{1}{4},y,x$

ORIGIN CHOICE 2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	Reflection conditions
							h,k,l permutable
							General:
192	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{4},\bar{y}+\frac{3}{4},z+\frac{1}{2}$	(3) $\bar{x}+\frac{3}{4},y+\frac{1}{2},\bar{z}+\frac{1}{4}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{4},\bar{z}+\frac{3}{4}$	hkl: $h+k=2n$ and $h+l,k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(7) $\bar{z}+\frac{1}{4},\bar{x}+\frac{3}{4},y+\frac{1}{2}$	(8) $\bar{z}+\frac{3}{4},x+\frac{1}{2},\bar{y}+\frac{1}{4}$	
			(9) y,z,x	(10) $\bar{y}+\frac{3}{4},z+\frac{1}{2},\bar{x}+\frac{1}{4}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(12) $\bar{y}+\frac{1}{4},\bar{z}+\frac{3}{4},x+\frac{1}{2}$	$0kl$: $k+l=4n$ and $k,l=2n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}$	(14) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(15) $y+\frac{1}{4},\bar{x},z+\frac{3}{4}$	(16) $\bar{y},x+\frac{3}{4},z+\frac{1}{4}$	
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}$	(18) $\bar{x},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2}$	(20) $x+\frac{1}{4},\bar{z},y+\frac{3}{4}$	hhl: $h,l=2n$
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}$	(22) $z+\frac{1}{4},\bar{y},x+\frac{3}{4}$	(23) $\bar{z},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$h00$: $h=4n$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{3}{4},y+\frac{1}{4},\bar{z}+\frac{1}{2}$	(27) $x+\frac{1}{4},\bar{y}+\frac{1}{2},z+\frac{3}{4}$	(28) $\bar{x}+\frac{1}{2},y+\frac{3}{4},z+\frac{1}{4}$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{3}{4},y+\frac{1}{4}$	(31) $z+\frac{3}{4},x+\frac{1}{4},\bar{y}+\frac{1}{2}$	(32) $z+\frac{1}{4},\bar{x}+\frac{1}{2},y+\frac{3}{4}$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y+\frac{1}{4},\bar{z}+\frac{1}{2},x+\frac{3}{4}$	(35) $\bar{y}+\frac{1}{2},z+\frac{3}{4},x+\frac{1}{4}$	(36) $y+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{1}{2}$	
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z$	(38) $y+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(39) $\bar{y}+\frac{3}{4},x,\bar{z}+\frac{1}{4}$	(40) $y,\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y$	(42) $x,\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) $x+\frac{1}{2},z+\frac{1}{2},y+\frac{1}{2}$	(44) $\bar{x}+\frac{3}{4},z,\bar{y}+\frac{1}{4}$	
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x$	(46) $\bar{z}+\frac{3}{4},y,\bar{x}+\frac{1}{4}$	(47) $z,\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) $z+\frac{1}{2},y+\frac{1}{2},x+\frac{1}{2}$	
							Special: as above, plus
96	g	. . 2	$\frac{1}{4},y,\bar{y}$	$0,\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2}$	$\frac{1}{2},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{3}{4},\bar{y}+\frac{1}{4},y+\frac{3}{4}$	no extra conditions
			$\bar{y},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},0,\bar{y}+\frac{3}{4}$	$y+\frac{1}{4},\frac{1}{2},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{4},\bar{y}+\frac{1}{4}$	
			$y,\bar{y},\frac{1}{4}$	$\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2},0$	$y+\frac{1}{2},y+\frac{1}{4},\frac{1}{2}$	$\bar{y}+\frac{1}{4},y+\frac{3}{4},\frac{3}{4}$	
			$\frac{3}{4},\bar{y},y$	$0,y+\frac{1}{4},y+\frac{1}{2}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{1}{4},y+\frac{3}{4},\bar{y}+\frac{1}{4}$	
			$y,\frac{3}{4},\bar{y}$	$y+\frac{1}{2},0,y+\frac{1}{4}$	$\bar{y}+\frac{3}{4},\frac{1}{2},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{4},\frac{1}{4},y+\frac{3}{4}$	
			$\bar{y},y,\frac{3}{4}$	$y+\frac{1}{4},y+\frac{1}{2},0$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{1}{2}$	$y+\frac{3}{4},\bar{y}+\frac{1}{4},\frac{1}{4}$	
96	f	2 . .	$x,\frac{1}{8},\frac{1}{8}$	$\bar{x}+\frac{1}{4},\frac{5}{8},\frac{5}{8}$	$\frac{1}{8},x,\frac{1}{8}$	$\frac{5}{8},\bar{x}+\frac{1}{4},\frac{5}{8}$	hkl: $h+k+l=4n$
			$\frac{7}{8},x+\frac{1}{4},\frac{7}{8}$	$\frac{3}{8},\bar{x}+\frac{1}{2},\frac{3}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{7}{8}$	$\bar{x},\frac{7}{8},\frac{3}{8}$	
			$\bar{x},\frac{7}{8},\frac{7}{8}$	$x+\frac{3}{4},\frac{3}{8},\frac{3}{8}$	$\frac{7}{8},\bar{x},\frac{7}{8}$	$\frac{3}{8},x+\frac{3}{4},\frac{3}{8}$	
			$\frac{1}{8},\bar{x}+\frac{3}{4},\frac{1}{8}$	$\frac{5}{8},x+\frac{1}{2},\frac{5}{8}$	$\bar{x}+\frac{1}{4},\frac{5}{8},\frac{1}{8}$	$x,\frac{1}{8},\frac{5}{8}$	
			$\frac{1}{8},\frac{1}{8},x$	$\frac{5}{8},\frac{5}{8},\bar{x}+\frac{1}{4}$			
			$\frac{7}{8},\frac{3}{8},\bar{x}$	$\frac{3}{8},\frac{7}{8},x+\frac{3}{4}$			
			$\frac{7}{8},\frac{7}{8},\bar{x}$	$\frac{3}{8},\frac{3}{8},x+\frac{3}{4}$			
			$\frac{1}{8},\frac{5}{8},x$	$\frac{5}{8},\frac{1}{8},\bar{x}+\frac{1}{4}$			
64	e	. 3 .	x,x,x	$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{1}{2}$	$\bar{x}+\frac{3}{4},x+\frac{1}{2},\bar{x}+\frac{1}{4}$	$x+\frac{1}{2},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$	hkl: $h=2n$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{4},\bar{x},x+\frac{3}{4}$	$\bar{x},x+\frac{3}{4},x+\frac{1}{4}$	
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{2}$	$x+\frac{1}{4},\bar{x}+\frac{1}{2},x+\frac{3}{4}$	$\bar{x}+\frac{1}{2},x+\frac{3}{4},x+\frac{1}{4}$	
			$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x$	$x+\frac{1}{2},x+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{3}{4},x,\bar{x}+\frac{1}{4}$	$x,\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$	
48	d	$\bar{4}$ . .	$\frac{7}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{5}{8},\frac{5}{8}$	$\frac{1}{8},\frac{7}{8},\frac{1}{8}$	$\frac{5}{8},\frac{3}{8},\frac{5}{8}$	hkl: $h+k+l=4n$
			$\frac{7}{8},\frac{1}{8},\frac{7}{8}$	$\frac{3}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	$\frac{1}{8},\frac{7}{8},\frac{3}{8}$	
			$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{7}{8},\frac{1}{8},\frac{3}{8}$			
			$\frac{7}{8},\frac{3}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$			
32	c	. $\bar{3}$.	$0,0,0$	$\frac{1}{4},\frac{3}{4},\frac{1}{2}$	$\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\frac{3}{4}$	hkl: $h,k,l=4n+2$ or $h,k,l=4n$
			$\frac{3}{4},\frac{1}{4},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},0,\frac{3}{4}$	$0,\frac{3}{4},\frac{1}{4}$	
32	b	. 3 2	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},0$	$\frac{3}{4},0,\frac{1}{2}$	hkl: $h,k,l=4n+2$ or $h,k,l=4n$
			$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{4},0,\frac{1}{2}$	
16	a	2 3 .	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{7}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{1}{8},\frac{5}{8},\frac{1}{8}$	hkl: $h+k+l=4n$



Symmetry of special projections

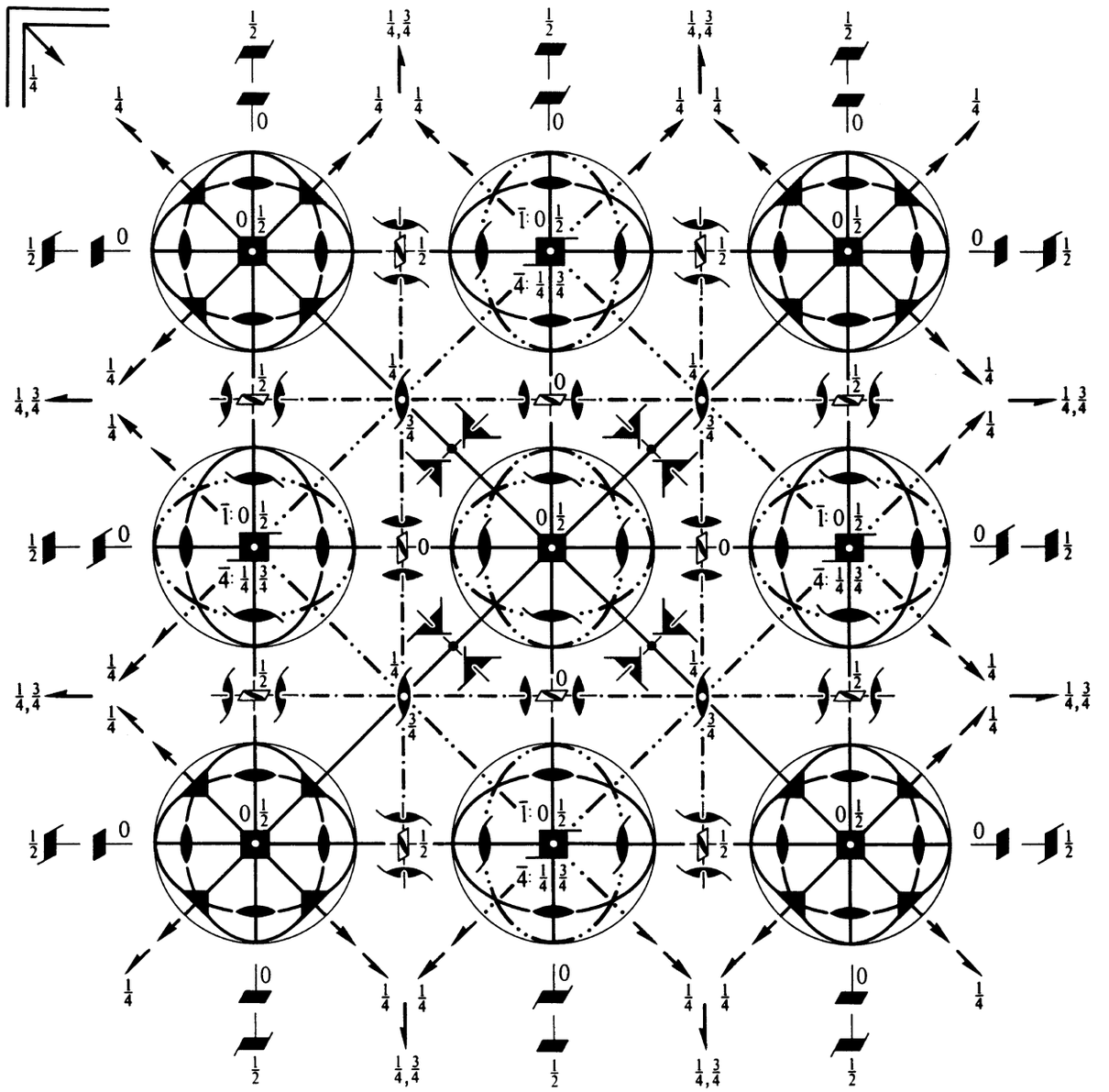
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{4}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{4}(\mathbf{a}+\mathbf{b})$
Origin at $\frac{1}{8},\frac{3}{8},z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{6}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{6}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{4}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$I\,m\bar{3}\,m$ O_h^9 $m\bar{3}\,m$ Cubic

No. 229 $I\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $I\,m\bar{3}\,m$



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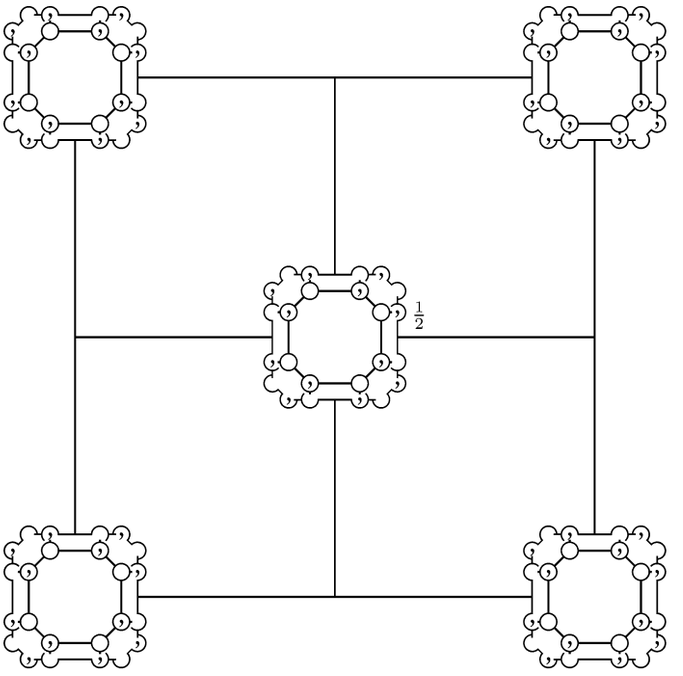


Origin at centre $(m\bar{3}m)$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{4}$; $y \le x$; $z \le \min(\frac{1}{2}-x, y)$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{1}{2},\frac{1}{2},0$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) 2 0,0,z	(3) 2 0,y,0	(4) 2 x,0,0
(5) 3^+ x,x,x	(6) 3^+ $\bar{x},x,\bar{x}$	(7) 3^+ $x,\bar{x},\bar{x}$	(8) 3^+ $\bar{x},\bar{x},x$
(9) 3^- x,x,x	(10) 3^- $x,\bar{x},\bar{x}$	(11) 3^- $\bar{x},\bar{x},x$	(12) 3^- $\bar{x},x,\bar{x}$
(13) 2 x,x,0	(14) 2 $x,\bar{x}$,0	(15) 4^- 0,0,z	(16) 4^+ 0,0,z
(17) 4^- x,0,0	(18) 2 0,y,y	(19) 2 0,$y,\bar{y}$	(20) 4^+ x,0,0
(21) 4^+ 0,y,0	(22) 2 x,0,x	(23) 4^- 0,y,0	(24) 2 $\bar{x}$,0,x
(25) $\bar{1}$ 0,0,0	(26) m x,y,0	(27) m x,0,z	(28) m 0,y,z
(29) $\bar{3}^+$ x,x,x; 0,0,0	(30) $\bar{3}^+$ $\bar{x},x,\bar{x}$; 0,0,0	(31) $\bar{3}^+$ $x,\bar{x},\bar{x}$; 0,0,0	(32) $\bar{3}^+$ $\bar{x},\bar{x},x$; 0,0,0
(33) $\bar{3}^-$ x,x,x; 0,0,0	(34) $\bar{3}^-$ $x,\bar{x},\bar{x}$; 0,0,0	(35) $\bar{3}^-$ $\bar{x},\bar{x},x$; 0,0,0	(36) $\bar{3}^-$ $\bar{x},x,\bar{x}$; 0,0,0
(37) m $x,\bar{x},z$	(38) m x,x,z	(39) $\bar{4}^-$ 0,0,z; 0,0,0	(40) $\bar{4}^+$ 0,0,z; 0,0,0
(41) $\bar{4}^-$ x,0,0; 0,0,0	(42) m $x,y,\bar{y}$	(43) m x,y,y	(44) $\bar{4}^+$ x,0,0; 0,0,0
(45) $\bar{4}^+$ 0,y,0; 0,0,0	(46) m $\bar{x},y,x$	(47) $\bar{4}^-$ 0,y,0; 0,0,0	(48) m x,y,x

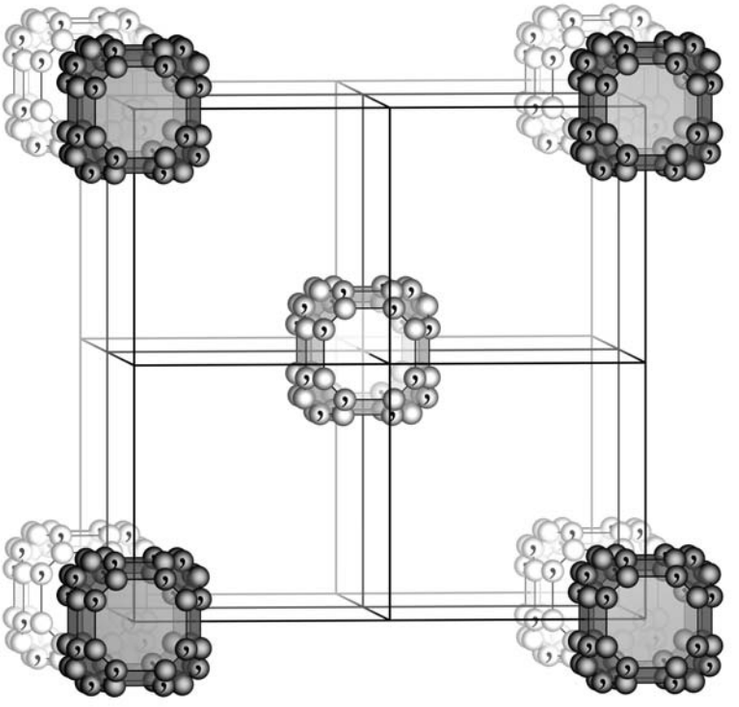
For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},x+\frac{1}{3},\bar{x}$	(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{2}{3},\bar{x}-\frac{1}{3},\bar{x}$	(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{2}{3},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x	(10) $3^-(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{3},\bar{x}+\frac{1}{3},\bar{x}$	(11) $3^-(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{2}{3},\bar{x}+\frac{1}{3},x$	(12) $3^-(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{3},x+\frac{2}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x,\frac{1}{4}$	(14) 2 $x,\bar{x}+\frac{1}{2},\frac{1}{4}$	(15) $4^-(0,0,\frac{1}{2})$ $\frac{1}{2}$,0,z	(16) $4^+(0,0,\frac{1}{2})$ $0,\frac{1}{2},z$
(17) $4^-(\frac{1}{2},0,0)$ $x,\frac{1}{2},0$	(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,y$	(19) 2 $\frac{1}{4},y+\frac{1}{2},\bar{y}$	(20) $4^+(\frac{1}{2},0,0)$ $x,0,\frac{1}{2}$
(21) $4^+(0,\frac{1}{2},0)$ $\frac{1}{2},y,0$	(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},x$	(23) $4^-(0,\frac{1}{2},0)$ $0,y,\frac{1}{2}$	(24) 2 $\bar{x}+\frac{1}{2},\frac{1}{4},x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(26) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(27) $n(\frac{1}{2},0,\frac{1}{2})$ $x,\frac{1}{4},z$	(28) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$
(29) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(30) $\bar{3}^+$ $\bar{x}-1,x+1,\bar{x}$; $-\frac{1}{4},\frac{1}{4},\frac{3}{4}$	(31) $\bar{3}^+$ $x,\bar{x}+1,\bar{x}$; $\frac{1}{4},\frac{3}{4},-\frac{1}{4}$	(32) $\bar{3}^+$ $\bar{x}+1,\bar{x},x$; $\frac{3}{4},-\frac{1}{4},\frac{1}{4}$
(33) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	(34) $\bar{3}^-$ $x+1,\bar{x}-1,\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{3}{4}$	(35) $\bar{3}^-$ $\bar{x},\bar{x}+1,x$; $-\frac{1}{4},\frac{3}{4},\frac{1}{4}$	(36) $\bar{3}^-$ $\bar{x}+1,x,\bar{x}$; $\frac{3}{4},\frac{1}{4},-\frac{1}{4}$
(37) c $x+\frac{1}{2},\bar{x},z$	(38) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,z	(39) $\bar{4}^-$ 0,$\frac{1}{2},z$; 0,$\frac{1}{2},\frac{1}{4}$	(40) $\bar{4}^+$ $\frac{1}{2}$,0,z; $\frac{1}{2}$,0,$\frac{1}{4}$
(41) $\bar{4}^-$ x,0,$\frac{1}{2}$; $\frac{1}{4}$,0,$\frac{1}{2}$	(42) a $x,y+\frac{1}{2},\bar{y}$	(43) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,y	(44) $\bar{4}^+$ $x,\frac{1}{2}$,0; $\frac{1}{4},\frac{1}{2}$,0
(45) $\bar{4}^+$ 0,$y,\frac{1}{2}$; 0,$\frac{1}{4},\frac{1}{2}$	(46) b $\bar{x}+\frac{1}{2},y,x$	(47) $\bar{4}^-$ $\frac{1}{2},y$,0; $\frac{1}{2},\frac{1}{4}$,0	(48) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,y,x

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$						Reflection conditions
									h,k,l permutable General:
96	l	1	(1) x,y,z (5) z,x,y (9) y,z,x (13) $y,x,\bar{z}$ (17) $x,z,\bar{y}$ (21) $z,y,\bar{x}$ (25) $\bar{x},\bar{y},\bar{z}$ (29) $\bar{z},\bar{x},\bar{y}$ (33) $\bar{y},\bar{z},\bar{x}$ (37) $\bar{y},\bar{x},z$ (41) $\bar{x},\bar{z},y$ (45) $\bar{z},\bar{y},x$	(2) $\bar{x},\bar{y},z$ (6) $z,\bar{x},\bar{y}$ (10) $\bar{y},z,\bar{x}$ (14) $\bar{y},\bar{x},\bar{z}$ (18) $\bar{x},z,y$ (22) $z,\bar{y},x$ (26) $x,y,\bar{z}$ (30) $\bar{z},x,y$ (34) $y,\bar{z},x$ (38) y,x,z (42) $x,\bar{z},\bar{y}$ (46) $\bar{z},y,\bar{x}$	(3) $\bar{x},y,\bar{z}$ (7) $\bar{z},\bar{x},y$ (11) $y,\bar{z},\bar{x}$ (15) $y,\bar{x},z$ (19) $\bar{x},\bar{z},\bar{y}$ (23) $\bar{z},y,x$ (27) $x,\bar{y},z$ (31) $z,x,\bar{y}$ (35) $\bar{y},z,x$ (39) $\bar{y},x,\bar{z}$ (43) x,z,y (47) $z,\bar{y},\bar{x}$	(4) $x,\bar{y},\bar{z}$ (8) $\bar{z},x,\bar{y}$ (12) $\bar{y},\bar{z},x$ (16) $\bar{y},x,z$ (20) $x,\bar{z},y$ (24) $\bar{z},\bar{y},\bar{x}$ (28) $\bar{x},y,z$ (32) $z,\bar{x},y$ (36) $y,z,\bar{x}$ (40) $y,\bar{x},\bar{z}$ (44) $\bar{x},z,\bar{y}$ (48) z,y,x			hkl: $h+k+l=2n$ $0kl$: $k+l=2n$ hhl: $l=2n$ $h00$: $h=2n$
									Special: as above, plus
48	k	$..m$	x,x,z $\bar{z},\bar{x},x$ $x,x,\bar{z}$ $\bar{x},\bar{z},\bar{x}$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{z},x$	$\bar{x},x,\bar{z}$ x,z,x $x,\bar{x},z$ $z,x,\bar{x}$	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$ $\bar{x},x,z$ $z,\bar{x},x$	z,x,x $x,\bar{z},\bar{x}$ $x,z,\bar{x}$ $\bar{z},x,x$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$ $\bar{x},z,x$ $\bar{z},\bar{x},\bar{x}$	no extra conditions
48	j	$m..$	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$ $0,z,y$ $\bar{z},\bar{y},0$	no extra conditions
48	i	$..2$	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},y$ $y,\bar{y}+\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},\bar{y},y+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y},y+\frac{1}{2},\frac{3}{4}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$ $\frac{1}{4},y,y+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},y$ $y,y+\frac{1}{2},\frac{1}{4}$	$\frac{3}{4},y,y+\frac{1}{2}$ $y+\frac{1}{2},\frac{3}{4},y$ $y,y+\frac{1}{2},\frac{3}{4}$ $\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$ $\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$ $y+\frac{1}{2},\frac{1}{4},\bar{y}$ $\bar{y},y+\frac{1}{2},\frac{1}{4}$ $\frac{3}{4},y,\bar{y}+\frac{1}{2}$ $\bar{y}+\frac{1}{2},\frac{3}{4},y$ $y,\bar{y}+\frac{1}{2},\frac{3}{4}$			no extra conditions
24	h	$m.m2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$	no extra conditions
24	g	$mm2..$	$x,0,\frac{1}{2}$ $0,x,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$ $0,\bar{x},\frac{1}{2}$	$\frac{1}{2},x,0$ $x,\frac{1}{2},0$	$\frac{1}{2},\bar{x},0$ $\bar{x},\frac{1}{2},0$	$0,\frac{1}{2},x$ $\frac{1}{2},0,\bar{x}$	$0,\frac{1}{2},\bar{x}$ $\frac{1}{2},0,x$	no extra conditions
16	f	$.3\,m$	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$			no extra conditions
12	e	$4\,m\,.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	no extra conditions
12	d	$\bar{4}\,m\,.2$	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	no extra conditions
8	c	$.\bar{3}\,m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$			hkl: $k,l=2n$
6	b	$4/m\,m\,.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$				no extra conditions
2	a	$m\bar{3}\,m$	$0,0,0$						no extra conditions



Symmetry of special projections

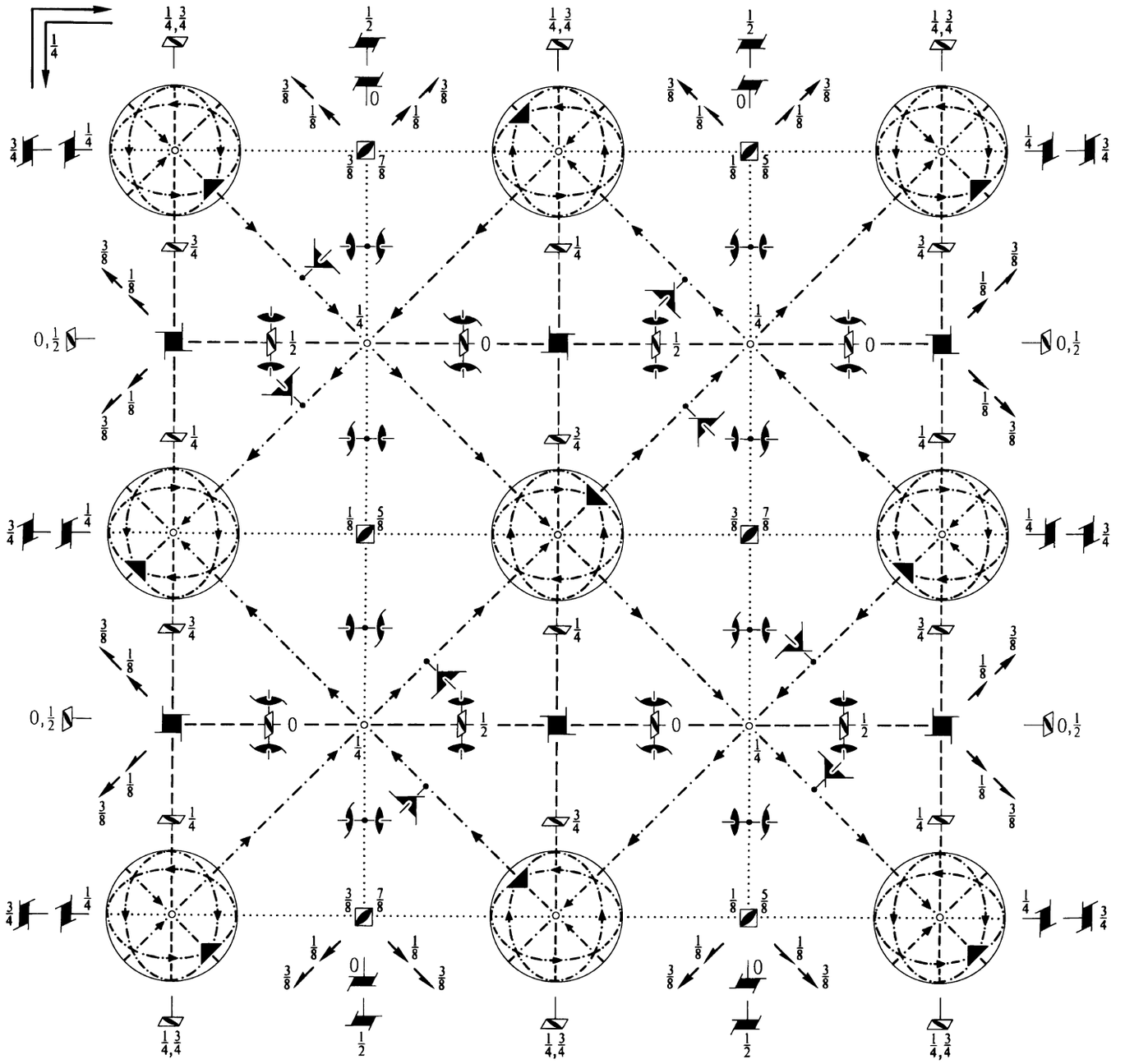
Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}(\mathbf{a}-\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Origin at $0,0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $p2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x,0$

$I\,a\,\bar{3}\,d$ O_h^{10} $m\bar{3}m$ Cubic

No. 230 $I\ 4_1/a\ \bar{3}\ 2/d$ Patterson symmetry $Im\bar{3}m$



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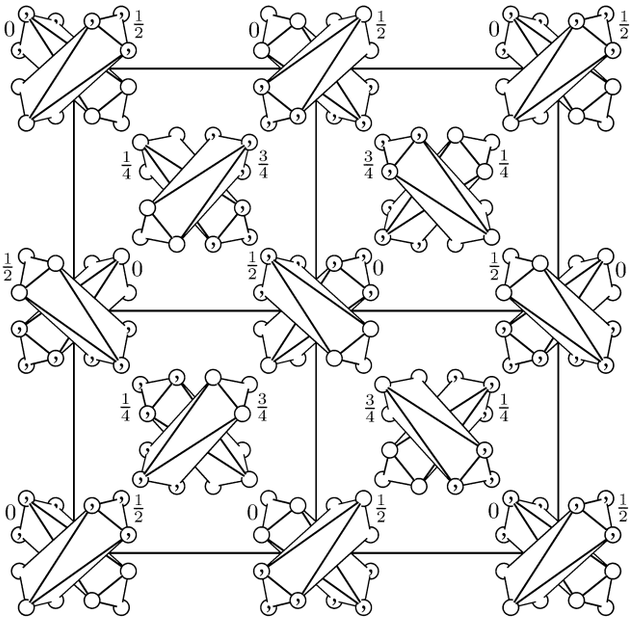
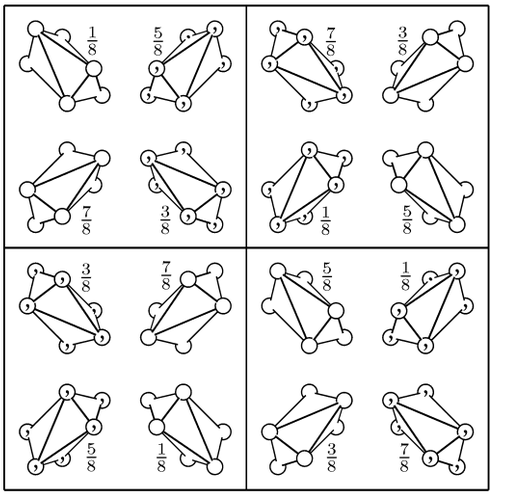


Polyhedron centre at 0, 0, 0



Polyhedron centre at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$

Origin at centre $(\bar{3})$

Asymmetric unit $-\frac{1}{8} \le x \le \frac{1}{8}$; $-\frac{1}{8} \le y \le \frac{1}{8}$; $0 \le z \le \frac{1}{4}$; $\max(x,-x,y,-y) \le z$

Vertices $0,0,0$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $-\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $-\frac{1}{8},-\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},-\frac{1}{8},\frac{1}{8}$
$\frac{1}{8},\frac{1}{8},\frac{1}{4}$ $-\frac{1}{8},\frac{1}{8},\frac{1}{4}$ $-\frac{1}{8},-\frac{1}{8},\frac{1}{4}$ $\frac{1}{8},-\frac{1}{8},\frac{1}{4}$

Symmetry operations

For (0,0,0)+ set

(1) 1
(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$
(3) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$
(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) 3^+ x,x,x
(6) 3^+ $\bar{x}+\frac{1}{2},x,\bar{x}$
(7) 3^+ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$
(8) 3^+ $\bar{x},\bar{x}+\frac{1}{2},x$
(9) 3^- x,x,x
(10) $3^-(-\frac{1}{3},\frac{1}{3},\frac{1}{3})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^-(\frac{1}{3},\frac{1}{3},-\frac{1}{3})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^-(\frac{1}{3},-\frac{1}{3},\frac{1}{3})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x-\frac{1}{4},\frac{1}{8}$
(14) 2 $x,\bar{x}+\frac{3}{4},\frac{3}{8}$
(15) $4^-(0,0,\frac{3}{4})$ $\frac{1}{4},0,z$
(16) $4^+(0,0,\frac{1}{4})$ $-\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{3}{4},0,0)$ $x,\frac{1}{4},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{8},y+\frac{1}{4},y$
(19) 2 $\frac{3}{8},y+\frac{3}{4},\bar{y}$
(20) $4^+(\frac{1}{4},0,0)$ $x,-\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{1}{4},0)$ $\frac{1}{2},y,-\frac{1}{4}$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x-\frac{1}{4},\frac{1}{8},x$
(23) $4^-(0,\frac{3}{4},0)$ $0,y,\frac{1}{4}$
(24) 2 $\bar{x}+\frac{3}{4},\frac{3}{8},x$
(25) $\bar{1}$ 0,0,0
(26) a $x,y,\frac{1}{4}$
(27) c $x,\frac{1}{4},z$
(28) b $\frac{1}{4},y,z$
(29) $\bar{3}^+$ x,x,x; 0,0,0
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x+1,\bar{x}$; $0,\frac{1}{2},\frac{1}{2}$
(31) $\bar{3}^+$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $\frac{1}{2},\frac{1}{2},0$
(32) $\bar{3}^+$ $\bar{x}+1,\bar{x}+\frac{1}{2},x$; $\frac{1}{2},0,\frac{1}{2}$
(33) $\bar{3}^-$ x,x,x; 0,0,0
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; $0,0,\frac{1}{2}$
(35) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; $0,\frac{1}{2},0$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{1}{2},0,0$
(37) $d(-\frac{1}{4},\frac{1}{4},\frac{3}{4})$ $x+\frac{1}{2},\bar{x},z$
(38) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,x,z
(39) $\bar{4}^-$ $0,\frac{3}{4},z$; $0,\frac{3}{4},\frac{1}{8}$
(40) $\bar{4}^+$ $\frac{1}{2},-\frac{1}{4},z$; $\frac{1}{2},-\frac{1}{4},\frac{3}{8}$
(41) $\bar{4}^-$ $x,0,\frac{3}{4}$; $\frac{1}{8},0,\frac{3}{4}$
(42) $d(\frac{3}{4},-\frac{1}{4},\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$
(43) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{2},-\frac{1}{4}$; $\frac{3}{8},\frac{1}{2},-\frac{1}{4}$
(45) $\bar{4}^+$ $-\frac{1}{4},y,\frac{1}{2}$; $-\frac{1}{4},\frac{3}{8},\frac{1}{2}$
(46) $d(\frac{1}{4},\frac{3}{4},-\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{3}{4},y,0$; $\frac{3}{4},\frac{1}{8},0$
(48) $d(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ x,y,x

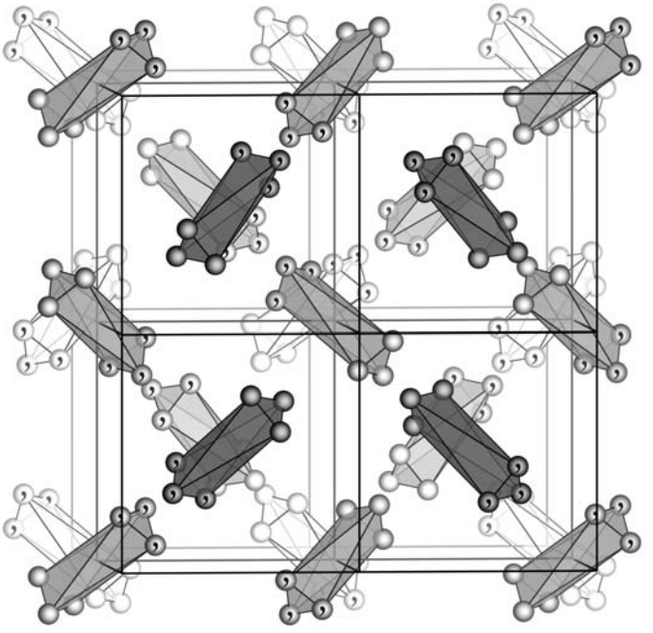
For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
(2) 2 $0,\frac{1}{4},z$
(3) 2 $\frac{1}{4},y,0$
(4) 2 $x,0,\frac{1}{4}$
(5) $3^+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x
(6) $3^+(\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(7) $3^+(-\frac{1}{6},\frac{1}{6},\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(8) $3^+(\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(9) $3^-(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ x,x,x
(10) $3^-(\frac{1}{6},-\frac{1}{6},-\frac{1}{6})$ $x+\frac{1}{6},\bar{x}+\frac{1}{6},\bar{x}$
(11) $3^-(-\frac{1}{6},-\frac{1}{6},\frac{1}{6})$ $\bar{x}+\frac{1}{3},\bar{x}+\frac{1}{6},x$
(12) $3^-(-\frac{1}{6},\frac{1}{6},-\frac{1}{6})$ $\bar{x}-\frac{1}{6},x+\frac{1}{3},\bar{x}$
(13) $2(\frac{1}{2},\frac{1}{2},0)$ $x,x+\frac{1}{4},\frac{3}{8}$
(14) 2 $x,\bar{x}+\frac{1}{4},\frac{1}{8}$
(15) $4^-(0,0,\frac{1}{4})$ $\frac{3}{4},0,z$
(16) $4^+(0,0,\frac{3}{4})$ $\frac{1}{4},\frac{1}{2},z$
(17) $4^-(\frac{1}{4},0,0)$ $x,\frac{3}{4},0$
(18) $2(0,\frac{1}{2},\frac{1}{2})$ $\frac{3}{8},y-\frac{1}{4},y$
(19) 2 $\frac{1}{8},y+\frac{1}{4},\bar{y}$
(20) $4^+(\frac{3}{4},0,0)$ $x,\frac{1}{4},\frac{1}{2}$
(21) $4^+(0,\frac{3}{4},0)$ $\frac{1}{2},y,\frac{1}{4}$
(22) $2(\frac{1}{2},0,\frac{1}{2})$ $x+\frac{1}{4},\frac{3}{8},x$
(23) $4^-(0,\frac{1}{4},0)$ $0,y,\frac{3}{4}$
(24) 2 $\bar{x}+\frac{1}{4},\frac{1}{8},x$
(25) $\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(26) b $x,y,0$
(27) a $x,0,z$
(28) c $0,y,z$
(29) $\bar{3}^+$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(30) $\bar{3}^+$ $\bar{x}-\frac{1}{2},x,\bar{x}$; $-\frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(31) $\bar{3}^+$ $x-\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$; $-\frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(32) $\bar{3}^+$ $\bar{x},\bar{x}-\frac{1}{2},x$; $\frac{1}{4},-\frac{1}{4},-\frac{1}{4}$
(33) $\bar{3}^-$ x,x,x; $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(34) $\bar{3}^-$ $x+\frac{1}{2},\bar{x}-\frac{1}{2},\bar{x}$; $\frac{1}{4},-\frac{1}{4},\frac{1}{4}$
(35) $\bar{3}^-$ $\bar{x},\bar{x}+\frac{1}{2},x$; $-\frac{1}{4},\frac{1}{4},\frac{1}{4}$
(36) $\bar{3}^-$ $\bar{x}+\frac{1}{2},x,\bar{x}$; $\frac{1}{4},\frac{1}{4},-\frac{1}{4}$
(37) $d(\frac{1}{4},-\frac{1}{4},\frac{1}{4})$ $x+\frac{1}{2},\bar{x},z$
(38) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,x,z
(39) $\bar{4}^-$ $0,\frac{1}{4},z$; $0,\frac{1}{4},\frac{3}{8}$
(40) $\bar{4}^+$ $\frac{1}{2},\frac{1}{4},z$; $\frac{1}{2},\frac{1}{4},\frac{1}{8}$
(41) $\bar{4}^-$ $x,0,\frac{1}{4}$; $\frac{3}{8},0,\frac{1}{4}$
(42) $d(\frac{1}{4},\frac{1}{4},-\frac{1}{4})$ $x,y+\frac{1}{2},\bar{y}$
(43) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,y,y
(44) $\bar{4}^+$ $x,\frac{1}{2},\frac{1}{4}$; $\frac{1}{8},\frac{1}{2},\frac{1}{4}$
(45) $\bar{4}^+$ $\frac{1}{4},y,\frac{1}{2}$; $\frac{1}{4},\frac{1}{8},\frac{1}{2}$
(46) $d(-\frac{1}{4},\frac{1}{4},\frac{1}{4})$ $\bar{x}+\frac{1}{2},y,x$
(47) $\bar{4}^-$ $\frac{1}{4},y,0$; $\frac{1}{4},\frac{3}{8},0$
(48) $d(\frac{3}{4},\frac{3}{4},\frac{3}{4})$ x,y,x

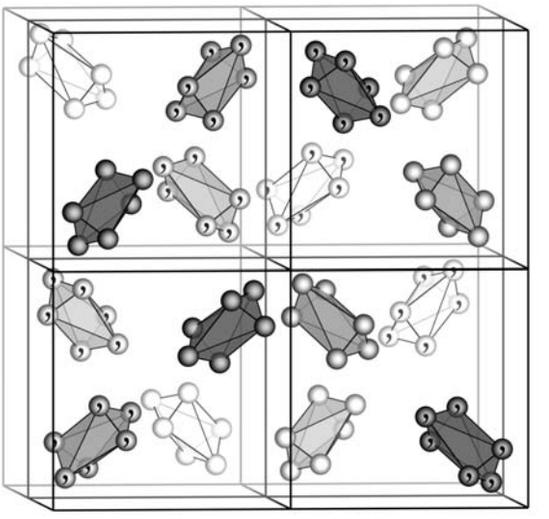
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				Reflection conditions
							h,k,l permutable
							General:
96	h	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	hkl: $h+k+l=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	$0kl$: $k,l=2n$
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	hhl: $2h+l=4n$
			(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{1}{4}$	(14) $\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{1}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{1}{4},x+\frac{3}{4},z+\frac{1}{4}$	$h00$: $h=4n$
			(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{1}{4}$	(18) $\bar{x}+\frac{1}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{3}{4},\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{1}{4},y+\frac{3}{4}$	
			(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{1}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{1}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{1}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{3}{4},\bar{y}+\frac{3}{4},\bar{x}+\frac{3}{4}$	
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(27) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(28) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(31) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(32) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(35) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(36) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	
			(37) $\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(38) $y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	(39) $\bar{y}+\frac{3}{4},x+\frac{3}{4},\bar{z}+\frac{1}{4}$	(40) $y+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4}$	
			(41) $\bar{x}+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$	(42) $x+\frac{3}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4}$	(43) $x+\frac{1}{4},z+\frac{1}{4},y+\frac{1}{4}$	(44) $\bar{x}+\frac{3}{4},z+\frac{3}{4},\bar{y}+\frac{1}{4}$	
			(45) $\bar{z}+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(46) $\bar{z}+\frac{3}{4},y+\frac{3}{4},\bar{x}+\frac{1}{4}$	(47) $z+\frac{3}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{3}{4}$	(48) $z+\frac{1}{4},y+\frac{1}{4},x+\frac{1}{4}$	
							Special: as above, plus
48	g	. . 2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{3}{8},\bar{y},\bar{y}+\frac{3}{4}$	$\frac{7}{8},y+\frac{1}{2},y+\frac{1}{4}$	$\frac{5}{8},\bar{y}+\frac{1}{2},y+\frac{3}{4}$	hkl: $h=2n+1$
			$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{3}{8},\bar{y}$	$y+\frac{1}{4},\frac{7}{8},y+\frac{1}{2}$	$y+\frac{3}{4},\frac{5}{8},\bar{y}+\frac{1}{2}$	or $h=4n$
			$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y},\bar{y}+\frac{3}{4},\frac{3}{8}$	$y+\frac{1}{2},y+\frac{1}{4},\frac{7}{8}$	$\bar{y}+\frac{1}{2},y+\frac{3}{4},\frac{5}{8}$	
			$\frac{7}{8},\bar{y},y+\frac{3}{4}$	$\frac{5}{8},y,y+\frac{1}{4}$	$\frac{1}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},\bar{y}+\frac{1}{4}$	
			$y+\frac{3}{4},\frac{7}{8},\bar{y}$	$y+\frac{1}{4},\frac{5}{8},y$	$\bar{y}+\frac{3}{4},\frac{1}{8},\bar{y}+\frac{1}{2}$	$\bar{y}+\frac{1}{4},\frac{3}{8},y+\frac{1}{2}$	
			$\bar{y},y+\frac{3}{4},\frac{7}{8}$	$y,y+\frac{1}{4},\frac{5}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{1}{8}$	$y+\frac{1}{2},\bar{y}+\frac{1}{4},\frac{3}{8}$	
48	f	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\frac{1}{4},x,0$	$\frac{3}{4},\bar{x}+\frac{1}{2},0$	$0,\frac{1}{4},x$	$0,\frac{3}{4},\bar{x}+\frac{1}{2}$	hkl: $2h+l=4n$
			$\frac{3}{4},x+\frac{1}{4},0$	$\frac{3}{4},\bar{x}+\frac{3}{4},\frac{1}{2}$	$x+\frac{3}{4},\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{4},0,\frac{1}{4}$	$0,\frac{1}{4},\bar{x}+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},x+\frac{3}{4}$	
			$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	$\frac{3}{4},\bar{x},0$	$\frac{1}{4},x+\frac{1}{2},0$	$0,\frac{3}{4},\bar{x}$	$0,\frac{1}{4},x+\frac{1}{2}$	
			$\frac{1}{4},\bar{x}+\frac{3}{4},0$	$\frac{1}{4},x+\frac{1}{4},\frac{1}{2}$	$\bar{x}+\frac{1}{4},\frac{1}{2},\frac{3}{4}$	$x+\frac{3}{4},0,\frac{3}{4}$	$0,\frac{3}{4},x+\frac{3}{4}$	$\frac{1}{2},\frac{3}{4},\bar{x}+\frac{1}{4}$	
32	e	. 3 .	x,x,x	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$	hkl: $h=2n+1$
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{1}{4}$	$\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4},\bar{x}+\frac{3}{4}$	$x+\frac{1}{4},\bar{x}+\frac{1}{4},x+\frac{3}{4}$	$\bar{x}+\frac{1}{4},x+\frac{3}{4},x+\frac{1}{4}$	or $h+k+l=4n$
			$\bar{x},\bar{x},\bar{x}$	$x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},x$	
			$\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$x+\frac{1}{4},x+\frac{1}{4},x+\frac{1}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},\bar{x}+\frac{1}{4}$	$x+\frac{3}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{3}{4}$	
24	d	$\bar{4}$ . .	$\frac{3}{8},0,\frac{1}{4}$	$\frac{1}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{3}{8},0$	$\frac{3}{4},\frac{1}{8},0$	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{1}{8}$	hkl: $h,k=2n$, $h+k+l=4n$
			$\frac{3}{4},\frac{5}{8},0$	$\frac{3}{4},\frac{3}{8},\frac{1}{2}$	$\frac{1}{8},\frac{1}{2},\frac{1}{4}$	$\frac{7}{8},0,\frac{1}{4}$	$0,\frac{1}{4},\frac{7}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	or $h,k=2n+1$, $l=4n+2$
									or $h=8n$, $k=8n+4$ and
24	c	2 . 2 2	$\frac{1}{8},0,\frac{1}{4}$	$\frac{3}{8},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{8},0$	$\frac{3}{4},\frac{3}{8},0$	$0,\frac{1}{4},\frac{1}{8}$	$0,\frac{3}{4},\frac{3}{8}$	$h+k+l=4n+2$
			$\frac{7}{8},0,\frac{3}{4}$	$\frac{5}{8},0,\frac{1}{4}$	$\frac{3}{4},\frac{7}{8},0$	$\frac{1}{4},\frac{5}{8},0$	$0,\frac{3}{4},\frac{7}{8}$	$0,\frac{1}{4},\frac{5}{8}$	
16	b	. 3 2	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{3}{8},\frac{7}{8},\frac{5}{8}$	$\frac{7}{8},\frac{5}{8},\frac{3}{8}$	$\frac{5}{8},\frac{3}{8},\frac{7}{8}$	$\frac{7}{8},\frac{7}{8},\frac{7}{8}$	$\frac{5}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{1}{8}$	hkl: $h,k=2n+1$, $l=4n+2$
											or $h,k,l=4n$
16	a	. $\bar{3}$.	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	hkl: $h,k=2n$, $h+k+l=4n$



Polyhedron centre at 0, 0, 0



Polyhedron centre at $\frac{1}{8},\frac{1}{8},\frac{1}{8}$

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}' = \frac{1}{2}\mathbf{a}$ $\mathbf{b}' = \frac{1}{2}\mathbf{b}$
Origin at $\frac{1}{4},0,z$

Along [111] $p6mm$
$\mathbf{a}' = \frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}' = \frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

Along [110] $c2mm$
$\mathbf{a}' = \frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}' = \frac{1}{2}\mathbf{c}$
Origin at $x,x+\frac{1}{4},\frac{1}{8}$

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3.1. Crystal lattices

H. Burzlaff, H. Grimmer, B. Gruber, P. M. de Wolff and H. Zimmermann

3.1.1. Bases and lattices

By H. Burzlaff and H. Zimmermann

3.1.1.1. Description and transformation of bases

In three dimensions, a coordinate system is defined by an origin and a basis consisting of three non-coplanar vectors. The lengths a, b, c of the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and the intervector angles $\alpha = \measuredangle(\mathbf{b}, \mathbf{c})$, $\beta = \measuredangle(\mathbf{c}, \mathbf{a})$, $\gamma = \measuredangle(\mathbf{a}, \mathbf{b})$ are called the *metric parameters*. In n dimensions, the lengths are designated a_i and the angles α_{ik}, where $1 \leq i < k \leq n$.

Another description of the basis consists of the scalar products of all pairs of basis vectors. The set of these scalar products obeys the rules of covariant tensors of the second rank (see Section 1.5.2). The scalar products may be written in the form of a (3×3) matrix

$$(\mathbf{a}_i \cdot \mathbf{a}_k) = (g_{ik}) = \boldsymbol{G}, \quad i, k = 1, 2, 3,$$

which is called the *matrix of the metric coefficients* or the *metric tensor*.

The change from one basis to another is described by a transformation matrix $\boldsymbol{P}$. The transformation of the old basis $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ to the new basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}')$ is given by

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c}) \cdot \boldsymbol{P}. \tag{3.1.1.1}$$

The relation

$$\boldsymbol{G}' = \boldsymbol{P}^{\mathrm{T}} \cdot \boldsymbol{G} \cdot \boldsymbol{P} \tag{3.1.1.2}$$

holds for the metric tensors $\boldsymbol{G}$ and $\boldsymbol{G}'$.

3.1.1.2. Lattices

A three-dimensional lattice can be visualized best as an infinite periodic array of points, which are the termini of the vectors

$$\mathbf{l}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}, \quad u, v, w \text{ all integers.}$$

The parallelepiped determined by the basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called a (primitive) *unit cell* of the lattice (*cf.* Section 1.3.2.3), $\mathbf{a}, \mathbf{b}$ and $\mathbf{c}$ are a primitive *basis of the lattice*. The number of possible lattice bases is infinite.

For the investigation of the properties of lattices, appropriate bases are required. In order to select suitable bases (see below), transformations may be necessary (Chapter 1.5). Of the several properties of lattices, only symmetry and some topological aspects are considered in this section. Some further properties of lattices are given in Section 3.1.4.

3.1.1.3. Topological properties of lattices

The treatment of the topological properties is restricted here to the consideration of the neighbourhood of a lattice point. For this purpose, the *domain of influence* (*Wirkungsbereich*, Dirichlet domain, Voronoi domain, Wigner–Seitz cell) (Delaunay, 1933) is introduced. The domain of a particular lattice point consists of all points in space that are closer to this lattice point than to any other lattice point or at most equidistant to it. To construct the domain, the selected lattice point is connected to all other lattice points. The set of planes perpendicular to these connecting lines and passing through their midpoints contains the boundary planes of the domain of influence, which is thus a convex polyhedron. (Niggli and Delaunay used the term 'domain of influence' for the interior of the convex polyhedron only.) Without the use of metrical properties, Minkowski (1897) proved that the maximal number of boundary planes resulting from this construction is equal to $2(2^n - 1)$, where n is the dimension of the space. The minimal number of boundary planes is $2n$. Each face of the polyhedron represents a lattice vector. Thus, the topological, metrical and symmetry properties of infinite lattices can be discussed with the aid of a single finite polyhedron, namely the domain of influence (*cf.* Burzlaff & Zimmermann, 1977).

3.1.1.4. Special bases for lattices

Different procedures are in use to select special bases of lattices. The reduction procedures employ metrical properties to develop a sequence of basis transformations which lead to a *reduced basis* and *reduced cell* (see Section 3.1.4).

Another possibility is to make use of the symmetry properties of lattices. This procedure, with the additional aid of standardization rules, leads to the *conventional crystallographic basis* and *cell*. In addition to translational symmetry, a lattice possesses point-group symmetry. No crystal can have higher point-group symmetry than the point group of its lattice, which is called its *holohedry*. (Detailed treatment of the symmetry properties of lattices and their classification is given in Chapter 1.3. Following the terminology introduced there, the lattice point groups are the geometric classes to which the Bravais groups of the lattices belong.) The seven holohedries in three dimensions and the four in two dimensions form the basis for the classification of lattices (Table 3.1.1.1). It may be shown by an algebraic approach (Burckhardt, 1966) or a topological one (Delaunay, 1933) that the arrangement of the symmetry elements with respect to the lattice vectors is not arbitrary but well determined. Taking as basis vectors lattice vectors along important symmetry directions and choosing the origin in a lattice point simplifies the description of the lattice symmetry operations (*cf.* Section 3.3.1). Note that such a basis is not necessarily a (primitive) basis of the lattice (see below). The choice of a basis controlled by symmetry is not always unique; in the monoclinic system, for example, one vector can be taken parallel to the symmetry direction but the other two vectors, perpendicular to it, are not uniquely determined by symmetry.

The choice of conventions for standardizing the setting of a lattice depends on the purpose for which it is used. The several sets of conventions rest on two conflicting principles: symmetry considerations and metric considerations. The following rules (i) to (vii) defining a *conventional basis* are taken from Donnay (1943; Donnay & Ondik, 1973); they deal with the conventions based on symmetry:

(i) Each basis vector is a lattice vector from the origin to the nearest node on the related row. The basis must define a right-handed coordinate system.

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Table 3.1.1.1
Lattice point-group symmetries

(*a*) Two dimensions.

Lattice point group	2	2*mm*	4*mm*	6*mm*
Crystal family†	*m*	*o*	*t*	*h*
	*m*onoclinic (oblique)	*o*rthorhombic (rectangular)	*t*etragonal (square)	*h*exagonal

(*b*) Three dimensions.

Lattice point group	$C_i \equiv \bar{1}$	$C_{2h} \equiv 2/m$	$D_{2h} \equiv mmm$	$D_{4h} \equiv 4/mmm$	$D_{3d} \equiv \bar{3}m$	$D_{6h} \equiv 6/mmm$	$O_h \equiv m\bar{3}m$
Crystal family†	*a*	*m*	*o*	*t*	*h*		*c*
	*a*northic (triclinic)	*m*onoclinic	*o*rthorhombic	*t*etragonal	*h*exagonal		*c*ubic

† The symbols for crystal families were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).

(ii) The basis vectors for a *cubic* lattice are parallel to the fourfold axes.

(iii*a*) In a *hexagonal* lattice, the basis vector parallel to the sixfold axis is labelled **c**. The remaining two basis vectors are taken along equivalent twofold axes and they must include an angle of 120°; from the two possible sets, the shorter vectors are chosen.

(iii*b*) For *rhombohedral* lattices, two descriptions are given in the present edition, as in earlier ones. The first description which results in the conventional cell uses 'hexagonal axes'. In this case, **c** is taken along the threefold axis. The remaining two vectors are chosen along equivalent twofold axes, which include an angle of 120°; they are oriented so that lattice points occur at $2/3, 1/3, 1/3$ and $1/3, 2/3, 2/3$ (obverse setting). The reverse setting ($0, 0, 0$; $1/3, 2/3, 1/3$; $2/3, 1/3, 2/3$) is not used in the space-group tables (*cf.* the second footnote to Table 2.1.1.2). The second description uses 'rhombohedral axes': **a**, **b** and **c** are the shortest three non-coplanar lattice vectors symmetry-equivalent with respect to the threefold axis.

(iv) In a *tetragonal* lattice, the vector **c** is along the fourfold axis, and **a** and **b** are chosen along equivalent twofold axes perpendicular to each other. From the two possible sets, the shorter vectors are chosen.

(v) In an *orthorhombic* lattice, **a**, **b** and **c** must be taken along the three twofold axes.

(vi) For *monoclinic* lattices, two 'settings' are given in the present edition. In one setting, the only symmetry direction is labelled **b** (*b*-unique setting). The basis vectors **a** and **c** are chosen to be the shortest two vectors in the net plane perpendicular to **b**, the angle β should be non-acute. This occurs if

$$0 \leq -2\mathbf{a} \cdot \mathbf{c} \leq \min(a^2, c^2). \qquad (3.1.1.3)$$

In the other setting, the symmetry direction is labelled **c** [*c*-unique setting; first introduced in *International Tables for X-ray Crystallography* (1952)]. In this case, **a** and **b** are the shortest two vectors in the net plane perpendicular to **c** and the angle γ should be non-acute. The *b*-unique setting is considered to be the standard setting.

(vii) The reduced basis is used to describe a *triclinic* (= *anorthic*) lattice (*cf.* Section 3.1.4).

The metric parameters of the conventional basis are called *lattice parameters*. For the purpose of identification, additional metric rules are to be applied to make the labelling unique; they can be found in the introduction to *Crystal Data* (Donnay & Ondik, 1973).

When the above rules have been applied, it may occur that not all lattice points can be described by integral coordinates. In such cases, the unit cell contains two, three or four lattice points. The additional points may be regarded as *centrings* of the conventional cell. They have simple rational coordinates. For a conventional basis, the number of lattice points per cell is 1, 2, 3 or 4 (see Tables 3.1.2.1 and 3.1.2.2).

In two dimensions, only two centring types are needed:

p: no centring (primitive);
c: face centred.

In three dimensions, the following centring types are used:

P: no centring (primitive);
I: body centred (*innenzentriert*);
F: all-face centred;
A, *B*, *C*: one-face centred, either (**b**, **c**) or (**c**, **a**) or (**a**, **b**);
R: hexagonal cell rhombohedrally centred [see rule (iii*b*) above].

In orthorhombic and monoclinic lattices, some differently centred cells can be transformed into each other without violating the symmetry conditions for the choice of the basis vectors. In these cases, the different centred cells belong to the same *centring mode*. In the orthorhombic case, the three types of one-face-centred cells belong to the same centring mode because the symbol of the cell depends only on the labelling of the basis vectors; *C* is usually preferred to *A* and *B* as the standard setting; the centring mode is designated *S* (*seitenflächenzentriert*). In the monoclinic case (*b*-unique setting), *A*, *I* and *C* may occur if the basis is chosen according to rule (vi). They can be transformed into each other without changing the symmetry direction. *C* is used for the standard setting (*cf.* Section 2.1.1.2); it represents the centring mode *S*. The vectors **a**, **c** are conventionally chosen as short as the *C*-centring allows so that they need not be the shortest two vectors in their net plane and need not fulfil the inequalities (3.1.1.3).

3.1.1.5. Remarks

(i) For the handling of special problems such as subgroup relations, it may be convenient to use additional types of centred cells, *e.g.* a hexagonal cell centred at $2/3, 1/3, 0$ and $1/3, 2/3, 0$, which is called *H*. In this case, rule (iii*a*) above is violated as vectors **a** and **b** are now directed along the second set of equivalent twofold axes. Similarly, for tetragonal

lattices, *C* may be used instead of *P*, or *F* instead of *I*; *cf.* Sections 1.5.4 and 2.1.1.2.

(ii) Readers who have studied Chapter 1.3 may realize that the 'lattice bases' defined here are also called 'primitive bases' and that both 'primitive bases' and 'conventional bases' are special cases of bases used in crystallography.

3.1.2. Bravais types of lattices and other classifications

By H. Burzlaff and H. Zimmermann

3.1.2.1. Classifications

By means of the above-mentioned lattice properties, it is possible to classify lattices according to various criteria. Lattices can be subdivided with respect to their topological types of domains, resulting in two classes in two dimensions and five classes in three dimensions. They are called *Voronoi types*. If the classification involves topological *and* symmetry properties of the domains, 24 *Symmetrische Sorten* (Delaunay, 1933) are obtained in three dimensions and 5 in two dimensions. Other classifications consider either the centring type or the point group of the lattice.

The most important classification takes into account both the lattice point-group symmetry and the centring mode (Bravais, 1866). The resulting classes are called *Bravais types of lattices* or, for short, *Bravais lattices*. Two lattices belong to the same Bravais type if and only if they coincide both in their point-group symmetry and in the centring mode of their conventional cells. The Bravais lattice characterizes the translational subgroup of a space group. The number of Bravais lattices is 1 in one dimension, 5 in two dimensions, 14 in three dimensions and 64 in four dimensions. The Bravais lattices may be derived by topological (Delaunay, 1933) or algebraic procedures (Burckhardt, 1966; Neubüser *et al.*, 1971). It can be shown (Wondratschek *et al.*, 1971) that 'all Bravais types of the same [crystal] family can be obtained from each other by the process of centring'. As a consequence, different Bravais types of the same crystal family (*cf.* Section 1.3.4) differ in their centring mode. Thus, the Bravais types may be described by a lower-case letter designating the crystal family and an upper-case letter designating the centring mode. The relations between the point groups of the lattices and the crystal families are shown in Table 3.1.1.1. Since the hexagonal and rhombohedral Bravais types belong to the same crystal family, the rhombohedral lattice is described by *hR*, *h* indicating the family and *R* the centring type. This nomenclature was adopted for the 1969 reprint of *International Tables for X-ray Crystallography* (1952) and for *Structure Reports* since 1975 (*cf.* Trotter, 1975).

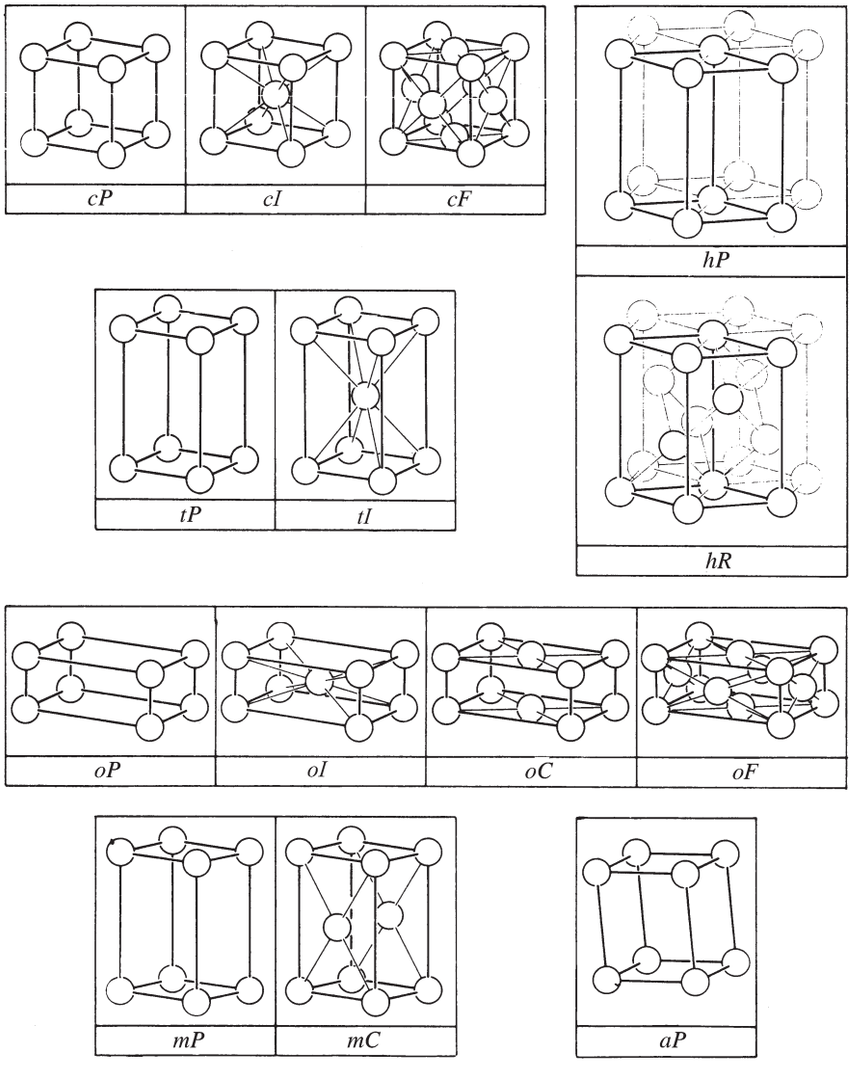


Figure 3.1.2.1
Conventional cells of the three-dimensional Bravais types of lattices (for symbols see Table 3.1.2.2).

3.1.2.2. Description of Bravais types of lattices

In Fig. 3.1.2.1, conventional cells for the 14 three-dimensional Bravais types of lattices are illustrated.

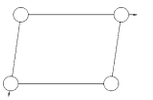
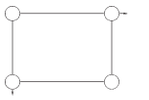
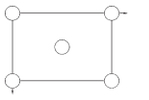
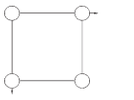
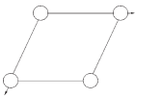
In Tables 3.1.2.1 and 3.1.2.2, the two- and three-dimensional Bravais types of lattices are described in detail. For each entry, the tables contain conditions that must be fulfilled by the lattice parameters and the metric tensor. These conditions are given with respect to two different basis systems, first the conventional basis related to symmetry, second a special primitive basis (see below). In columns 2 and 3, basis vectors not required by symmetry to be of the same length are designated by different letters. Columns 4 and 5 contain the metric tensors for the two related bases. Column 6 shows the relations between the components of the two tensors.

The last columns of Tables 3.1.2.1 and 3.1.2.2 show parallel projections of the appropriate conventional unit cells. Among the different possible choices of the primitive basis, as discussed in Section 3.1.1, the special primitive basis mentioned above is obtained according to the following rules:

(i) For each type of centring, only one transformation matrix $\boldsymbol{P}$ is used to obtain the primitive cell as given in Tables 3.1.2.1 and 3.1.2.2. The transformation obeys equation (3.1.1.2).

(ii) Among the different possible transformations, those are preferred which result in a metric tensor with simple relations among its components, as defined in Tables 3.1.2.1 and 3.1.2.2.

Table 3.1.2.1
Two-dimensional Bravais types of lattices

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/ transformation to primitive cell	Relations of the components	
mp	a, b γ	a, b γ	$g_{11}\ \ g_{12}$ $\ \ \ g_{22}$	$g_{11}\ \ g_{12}$ $\ \ \ g_{22}$		
op	a, b $\gamma = 90°$	a, b $\gamma = 90°$	$g_{11}\ \ 0$ $\ \ \ g_{22}$	$g_{11}\ \ 0$ $\ \ \ g_{22}$		
oc		$a_1 = a_2, \gamma$		$\boldsymbol{P}(c)$‡ $g'_{11}\ \ g'_{12}$ $\ \ \ g'_{11}$	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{12} = 2(g'_{11} - g'_{12})$	
tp	$a_1 = a_2$ $\gamma = 90°$	$a_1 = a_2$ $\gamma = 90°$	$g_{11}\ \ 0$ $\ \ \ g_{11}$	$g_{11}\ \ 0$ $\ \ \ g_{11}$		
hp	$a_1 = a_2$ $\gamma = 120°$	$a_1 = a_2$ $\gamma = 120°$	$g_{11}\ \ -\frac{1}{2}g_{11}$ $\ \ \ g_{11}$	$g_{11}\ \ -\frac{1}{2}g_{11}$ $\ \ \ g_{11}$		

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). ‡ $\boldsymbol{P}(c) = \frac{1}{2}(11/\bar{1}1)$.

If a primitive basis is chosen according to these rules, basis vectors of the conventional cell have parallel face-diagonal or body-diagonal orientation with respect to the basis vectors of the primitive cell. For cubic and rhombohedral lattices, the primitive basis vectors are selected such that they are symmetry-equivalent with respect to a threefold axis. In all cases, a face of the 'domain of influence' is perpendicular to each basis vector of these primitive cells.

3.1.2.3. Delaunay reduction and standardization

Further classifications use reduction theory. There are different approaches to the reduction of quadratic forms in mathematics. The two most important in our context are

(i) the Selling–Delaunay reduction (Selling, 1874),

(ii) the Eisenstein–Niggli reduction.

The investigations by Gruber (*cf.* Section 3.1.4) have shown the common root of both crystallographic approaches. As the Niggli reduction will be discussed in detail in Sections 3.1.3 and 3.1.4, we shall discuss the Delaunay reduction here.

We start with a lattice basis $(\mathbf{b}_i)_{1\le i\le n}$ $(n = 2, 3)$. This basis is extended by a vector

$$\mathbf{b}_{n+1} = -(\mathbf{b}_1 + \ldots + \mathbf{b}_n).$$

All scalar products

$$\mathbf{b}_i \cdot \mathbf{b}_k \ (1 \le i < k \le n+1)$$

are considered. The reduction is performed minimizing the sum

$$\sum = \mathbf{b}_1{}^2 + \ldots + \mathbf{b}_{n+1}{}^2.$$

It can be shown that this sum can be reduced by a sequence of transformations as long as one of the scalar products is still positive. If *e.g.* the scalar product $\mathbf{b}_1 \cdot \mathbf{b}_2$ is still positive, a transformation can be applied such that the sum $\sum'$ of the transformed $\mathbf{b}'^2_i$ is smaller than $\sum$:

$$\mathbf{b}'_1 = -\mathbf{b}_1,\ \mathbf{b}'_2 = \mathbf{b}_2,\ \mathbf{b}'_3 = \mathbf{b}_1 + \mathbf{b}_3 \text{ and } \mathbf{b}'_4 = \mathbf{b}_1 + \mathbf{b}_4.$$

In the two-dimensional case, $\mathbf{b}'_3 = 2\mathbf{b}_1 + \mathbf{b}_3$ holds.

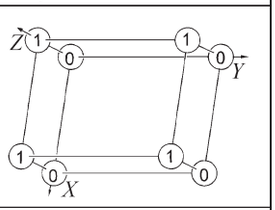
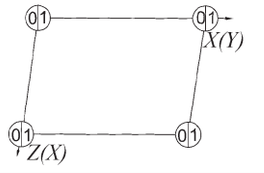
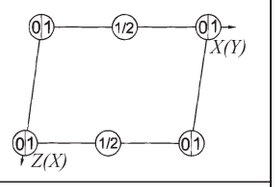
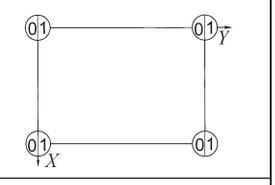
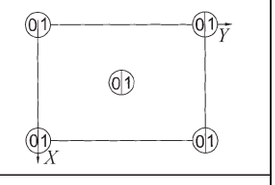
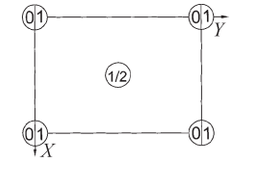
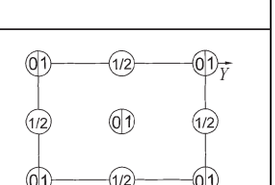
If all the scalar products are less than or equal to zero, the three shortest vectors of the reduced basis are contained in the set $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4, \mathbf{b}_1 + \mathbf{b}_2, \mathbf{b}_2 + \mathbf{b}_3, \mathbf{b}_3 + \mathbf{b}_1\}$, called the *Delaunay set*, which corresponds to the maximal set of faces of the Dirichlet domain (at most 14 faces).

The result of a reduction can be presented by a graphical symbol, the Selling tetrahedron. The four corners of the tetrahedron correspond to the vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3, \mathbf{b}_4$, the mutual scalar products are attached to the edges. A scalar product that is zero is indicated by '0'; equal scalar products are designated by the same graphical symbol (*cf.* Table 3.1.2.3).

Delaunay's classification is based on Voronoi types. Voronoi distinguishes five classes of Dirichlet domains. To describe these, the following symbols are used to represent particular topological features: s is used for a hexagon and for v for a quadrangle, s^2 indicates an edge between two hexagons and v^2 an edge between two quadrangles, v^4 is a vertex where four quadrangles meet and v^3 is a vertex where three quadrangles meet. The five types are topologically characterized by: V1 ($8s$, $6v$, $12s^2$), V2 ($4s$, $8v$, $4s^2$), V3 ($12v$, $24v^2$, $8v^3$, $6v^4$), V4 ($2s$, $6v$, $6v^2$) and V5 ($6v$, $12v^2$, $8v^3$). The numbers give the multiplicities of each feature.

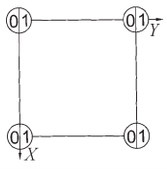
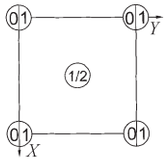
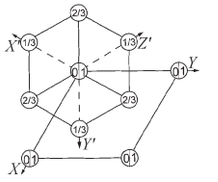
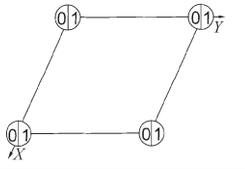
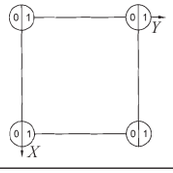
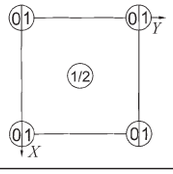
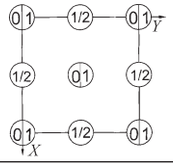
Delaunay combined the topological description with the rotation groups of the crystallographic holohedries. He used upper-case letters for these groups (K – cubic, H – hexagonal, R – rhombohedral, Q – tetragonal, O – orthorhombic, M – monoclinic, T – triclinic) followed by a incremental number if more than one Voronoi type with the same symmetry exists. The results are presented in Table 3.1.2.3. In each row a '*Symmetrische Sorte*' is described.

Table 3.1.2.2
Three-dimensional Bravais types of lattices

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.‡	Relations of the components	
aP	*a*, *b*, *c* α, β, γ	*a*, *b*, *c* α, β, γ	$g_{11}\ g_{12}\ g_{13}$ $g_{22}\ g_{23}$ g_{33}	$g_{11}\ g_{12}\ g_{13}$ $g_{22}\ g_{23}$ g_{33}		
mP	*a*, *b*, *c* β, $\alpha = \gamma = 90°$	*a*, *b*, *c* β, $\alpha = \gamma = 90°$	$g_{11}\ 0\ g_{13}$ $g_{22}\ 0$ g_{33}	$g_{11}\ 0\ g_{13}$ $g_{22}\ 0$ g_{33}		
mC (*mS*)		$a_1 = a_2$, *c* γ, $\alpha = \beta$		$\boldsymbol{P}(C)$ $g'_{11}\ g'_{12}\ g'_{13}$ $g'_{11}\ g'_{13}$ g_{33}	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g'_{13} = \frac{1}{2}g_{13}$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$ $g_{13} = 2g'_{13}$	
oP	*a*, *b*, *c* $\alpha = \beta = \gamma = 90°$	*a*, *b*, *c* $\alpha = \beta = \gamma = 90°$	$g_{11}\ 0\ 0$ $g_{22}\ 0$ g_{33}	$g_{11}\ 0\ 0$ $g_{22}\ 0$ g_{33}		
oC (*oS*)		$a_1 = a_2$, *c* γ, $\alpha = \beta = 90°$		$\boldsymbol{P}(C)$ $g'_{11}\ g'_{12}\ 0$ $g'_{11}\ 0$ g_{33}	$g'_{11} = \frac{1}{4}(g_{11} + g_{22})$ $g'_{12} = \frac{1}{4}(g_{11} - g_{22})$ $g_{11} = 2(g'_{11} + g'_{12})$ $g_{22} = 2(g'_{11} - g'_{12})$	
oI		$a_1 = a_2 = a_3$ α, β, γ $\cos\alpha + \cos\beta + \cos\gamma = -1$		$\boldsymbol{P}(I)$ $-\tilde{g}\ g'_{12}\ g'_{13}$ $-\tilde{g}\ g'_{23}$ $-\tilde{g}$ $\tilde{g} = g'_{12} + g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}(-g_{11} - g_{22} + g_{33})$ $g'_{13} = \frac{1}{4}(-g_{11} + g_{22} - g_{33})$ $g'_{23} = \frac{1}{4}(g_{11} - g_{22} - g_{33})$ $g_{11} = -2(g'_{12} + g'_{13})$ $g_{22} = -2(g'_{12} + g'_{23})$ $g_{33} = -2(g'_{13} + g'_{23})$	
oF		*a*, *b*, *c* α, β, γ $\cos\alpha = \dfrac{-a^2 + b^2 + c^2}{2bc}$ $\cos\beta = \dfrac{a^2 + b^2 + c^2}{2ac}$ $\cos\gamma = \dfrac{a^2 + b^2 - c^2}{2ab}$		$\boldsymbol{P}(F)$ $\tilde{g}_1\ g'_{12}\ g'_{13}$ $\tilde{g}_2\ g'_{23}$ $\tilde{g}_3$ $\tilde{g}_1 = g'_{12} + g'_{13}$ $\tilde{g}_2 = g'_{12} + g'_{23}$ $\tilde{g}_3 = g'_{13} + g'_{23}$	$g'_{12} = \frac{1}{4}g_{33}$ $g'_{13} = \frac{1}{4}g_{22}$ $g'_{23} = \frac{1}{4}g_{11}$ $g_{11} = 4g'_{23}$ $g_{22} = 4g'_{13}$ $g_{33} = 4g'_{12}$	

Column 1 contains the Delaunay description followed by the Voronoi type. Beneath these, the Bravais lattice and the symbol of its holohedry are given. Next the topological features that are compatible with the symmetry axes referred to the '*blickrichtungen*' of the holohedry are listed. Column 2 gives the metric conditions for the occurrence of certain Voronoi types. For the monoclinic cases with centred cells (*M*1–*M*5) it is useful to introduce in addition to the vectors **a**, **c**, **f** = **a** + **c** special parameters (p^2, q^2, r^2). **p** designates the vector below the centring point in the projection in the net perpendicular to **b**. **q** is the

Table 3.1.2.2 (continued)

Bravais type of lattice†	Lattice parameters		Metric tensor			Projections
	Conventional	Primitive	Conventional	Primitive/transf.‡	Relations of the components	
tP	$a_1 = a_2$, c $\alpha = \beta = \gamma = 90°$	$a_1 = a_2$, c $\alpha = \beta = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$		
tI		$a_1 = a_2 = a_3$ $\gamma, \alpha = \beta$ $2\cos\alpha + \cos\gamma = -1$		$\boldsymbol{P}(I)$ $\begin{matrix} \bar{g} & g'_{12} & g'_{13} \\ & \bar{g} & g'_{13} \\ & & \bar{g} \end{matrix}$ $\bar{g} = -(g'_{12} + 2g'_{13})$	$g'_{12} = \frac{1}{4}(-2g_{11} + g_{33})$ $g'_{13} = -\frac{1}{4}g_{33}$ $g_{11} = 2(g'_{12} + g'_{13})$ $g_{33} = -4g'_{13}$	
hR	$a_1 = a_2$, c $\alpha = \beta = 90°$ $\gamma = 120°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma$	$\begin{matrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$	$\boldsymbol{P}(R)$ $\begin{matrix} g'_{11} & g'_{12} & g'_{12} \\ & g'_{11} & g'_{12} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{1}{9}(3g_{11} + g_{33})$ $g'_{12} = \frac{1}{9}(-\frac{3}{2}g_{11} + g_{33})$ $g_{11} = 2(g'_{11} - g'_{12})$ $g_{33} = 3(g'_{11} + 2g'_{12})$	
hP		$a_1 = a_2$, c $\alpha = \beta = 90°$ $\gamma = 120°$		$\begin{matrix} g_{11} & -\frac{1}{2}g_{11} & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{matrix}$		
cP	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 90°$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{matrix}$	$\begin{matrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{matrix}$		
cI		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 109.5°$ $\cos\alpha = -\frac{1}{3}$		$\boldsymbol{P}(I)$ $\begin{matrix} g'_{11} & -\frac{1}{3}g'_{11} & -\frac{1}{3}g'_{11} \\ & g'_{11} & -\frac{1}{3}g'_{11} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{3}{4}g_{11}$ $g_{11} = \frac{4}{3}g'_{11}$	
cF		$a_1 = a_2 = a_3$ $\alpha = \beta = \gamma = 60°$		$\boldsymbol{P}(F)$ $\begin{matrix} g'_{11} & \frac{1}{2}g'_{11} & \frac{1}{2}g'_{11} \\ & g'_{11} & \frac{1}{2}g'_{11} \\ & & g'_{11} \end{matrix}$	$g'_{11} = \frac{1}{2}g_{11}$ $g_{11} = 2g'_{11}$	

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). Symbols in parentheses are standard symbols, see Table 2.1.1.1. ‡ $\boldsymbol{P}(C) = \frac{1}{2}(110/\bar{1}10/002)$, $\boldsymbol{P}(I) = \frac{1}{2}(\bar{1}11/1\bar{1}1/11\bar{1})$, $\boldsymbol{P}(F) = \frac{1}{2}(011/101/110)$, $\boldsymbol{P}(R) = \frac{1}{3}(\bar{1}21/\bar{2}11/111)$.

shorter one of the other two vectors and **r** labels the remaining one (*cf.* Burzlaff & Zimmermann, 1985).

For practical applications, it is useful to classify the patterns of the resulting six scalar products regarding their equivalence or zero values in the form of a symbolic (Selling) tetrahedron (column 3). These classes of patterns correspond to the reduced bases. They result in 24 '*Symmetrische Sorten*' (Delaunay, 1933) that fix the Voronoi types and the holohedries, and simultaneously lead directly to the conventional crystallographic cells by fixed transformations (*cf.* Patterson & Love, 1957; Burzlaff & Zimmermann, 1993).

Column 4 contains projections of the Dirichlet domain along the symmetry directions indicated by the topological/symmetry symbol in column 1. Column 5 shows the relation between the Dirichlet domain and the conventional cell. Column 6 contains the transformation matrix from the reduced basis to the conventional basis. (*Note*: In the monoclinic centred case it leads to the *I* centring.)

Table 3.1.2.3
Delaunay types of lattices (‘*Symmetrische Sorten*’)

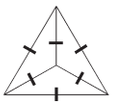
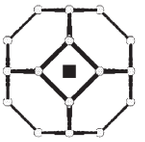
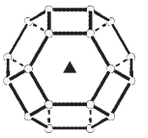
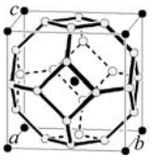
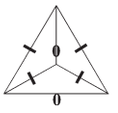
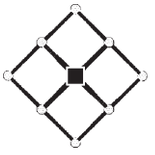
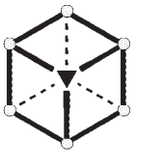
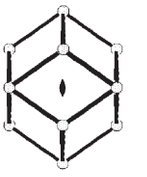
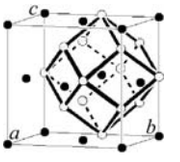
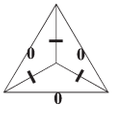
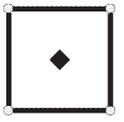
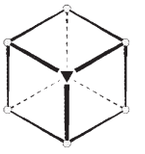
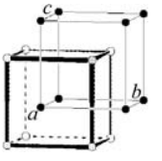
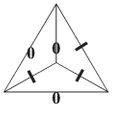
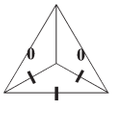
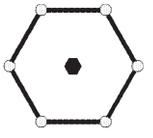
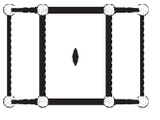
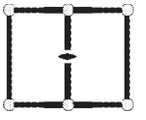
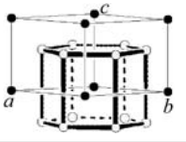
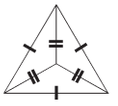
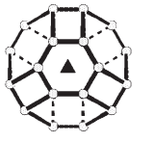
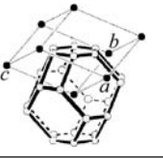
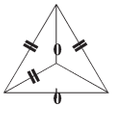
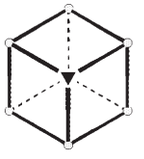
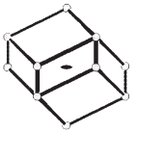
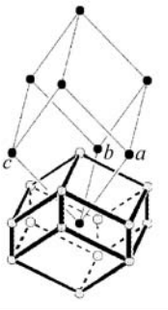
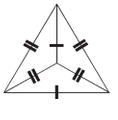
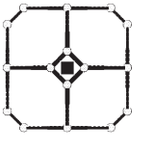
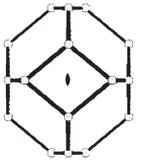
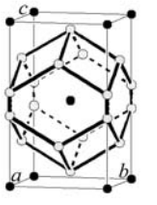
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
*K*1 V1 *cI* $\frac{4}{m}\bar{3}\frac{2}{m}$ *v s* s^2	–						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
*K*2 V3 *cF* $\frac{4}{m}\bar{3}\frac{2}{m}$ v^4 v^3 *v*	–						$\begin{pmatrix}1&-1&1\\1&1&1\\0&0&2\end{pmatrix}$
*K*3 V5 *cP* $\frac{4}{m}\bar{3}\frac{2}{m}$ *v* v^3 v^2	–						$\begin{pmatrix}1&0&0\\0&0&1\\0&1&1\end{pmatrix}$
							$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
H V4 *hP* $\frac{6}{m}\frac{2}{m}\frac{2}{m}$ *s v* v^2	–						$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
*R*1 V1 *hR* $\bar{3}\frac{2}{m}$ *s* s^2	$2c^2 < 3a^2$				–		$\begin{pmatrix}1&0&1\\-1&1&1\\0&-1&1\end{pmatrix}$
*R*2 V3 *hR* $\bar{3}\frac{2}{m}$ v^3 *v*	$2c^2 > 3a^2$				–		$\begin{pmatrix}1&0&1\\0&0&3\\0&1&2\end{pmatrix}$
*Q*1 V1 *tI* $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ *v v* s^2	$c^2 < 2a^2$						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$

Table 3.1.2.3 (continued)

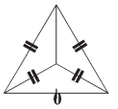
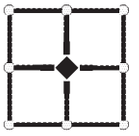
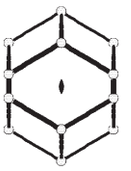
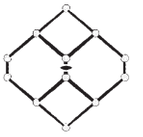
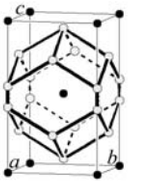
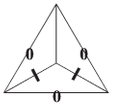
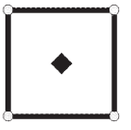
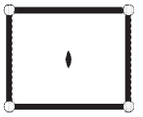
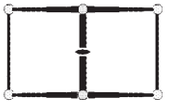
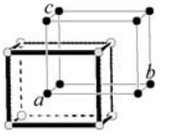
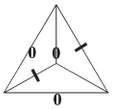
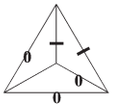
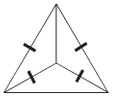
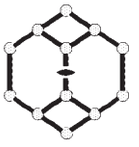
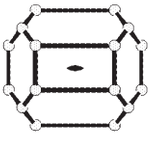
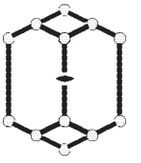
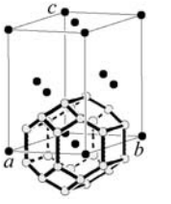
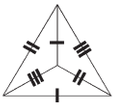
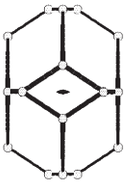
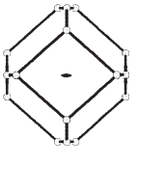
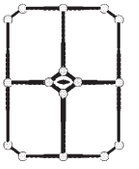
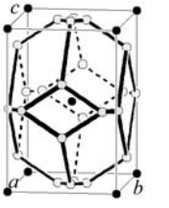
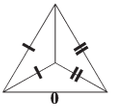
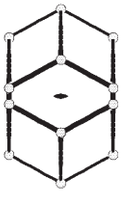
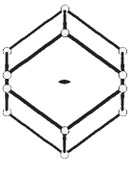
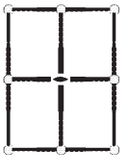
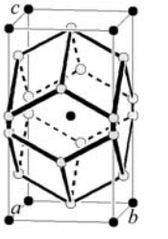
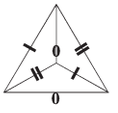
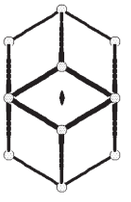
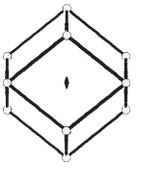
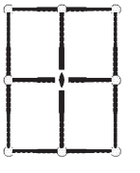
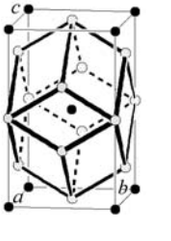
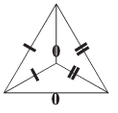
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
$Q2$ V2 tI $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ $v^4\ s\ s^2$	$c^2 > 2a^2$						$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$
$Q3$ V5 tP $\frac{4}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v^2$	–						$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
							$\begin{pmatrix}1&0&0\\0&0&1\\0&1&1\end{pmatrix}$
							$\begin{pmatrix}0&0&1\\1&1&0\\0&1&0\end{pmatrix}$
$O1$ V1 oF $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $s^2\ v\ s^2$	–						$\begin{pmatrix}1&-1&1\\1&1&1\\0&0&2\end{pmatrix}$
$O2$ V1 oI $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v$	$a^2 + b^2 > c^2$						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
$O3$ V2 oI $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $s\ s\ v^4$	$a^2 + b^2 < c^2$						$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$
$O4$ V3 oI $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ $v\ v\ v^4$	$a^2 + b^2 = c^2$						$\begin{pmatrix}0&1&1\\1&0&1\\1&1&0\end{pmatrix}$
							$\begin{pmatrix}1&0&1\\0&1&1\\0&0&2\end{pmatrix}$

Table 3.1.2.3 (continued)

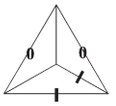
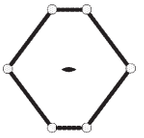
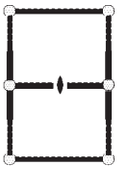
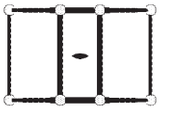
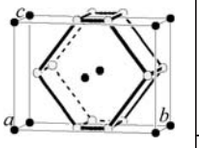
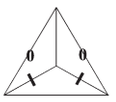
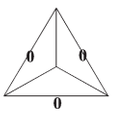
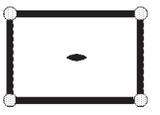
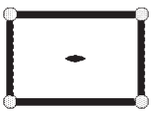
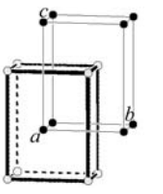
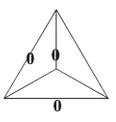
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions			Dirichlet domain in the unit cell	Transformation to the conventional cell
*O*5 V4 *o*(*AB*)*C* $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ *s* v^2 *v*	–						$\begin{pmatrix}2&0&0\\1&1&0\\0&0&1\end{pmatrix}$
							$\begin{pmatrix}1&1&0\\-1&1&0\\0&0&1\end{pmatrix}$
*O*6 V5 *oP* $\frac{2}{m}\frac{2}{m}\frac{2}{m}$ *v v v*	–						$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$
							$\begin{pmatrix}1&0&0\\0&0&1\\0&1&1\end{pmatrix}$

Table 3.1.2.3 (continued)

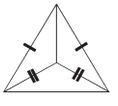
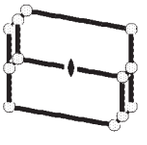
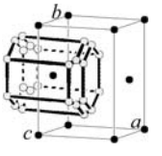
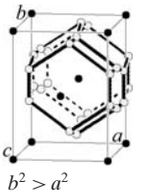
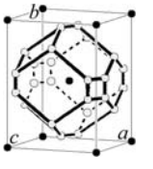
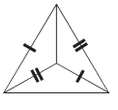
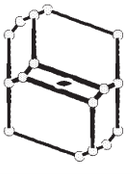
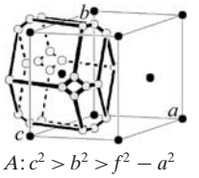
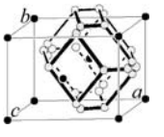
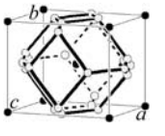
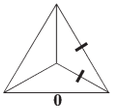
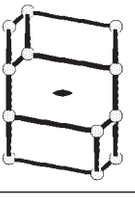
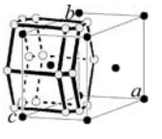
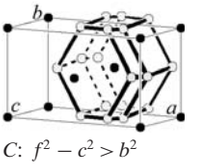
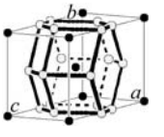
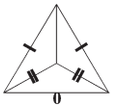
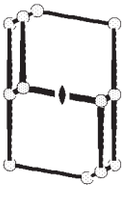
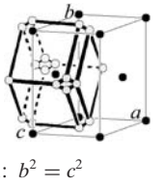
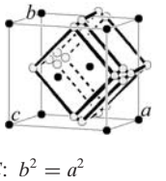
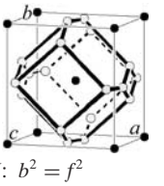
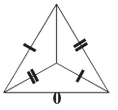
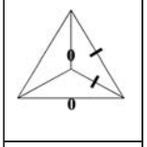
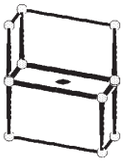
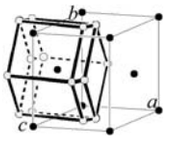
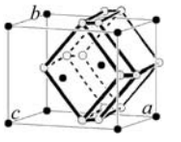
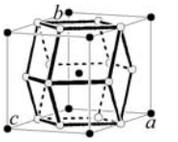
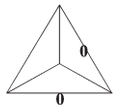
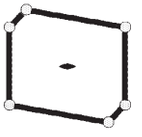
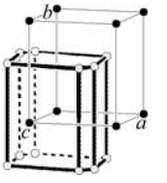
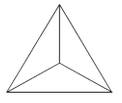
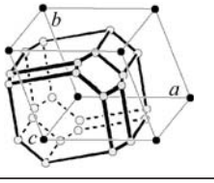
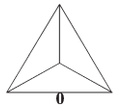
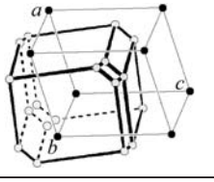
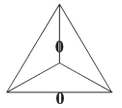
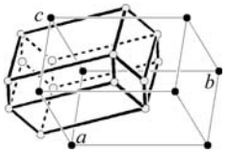
Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions	Dirichlet domain in the unit cell			Transformation to the conventional cell
*M*1 V1 *m*(*AC*)*I* $\frac{2}{m}$ s^2	$b^2 > p^2$			 *A*: $b^2 > c^2$	 *C*: $b^2 > a^2$	 *I*: $b^2 > f^2$	$\begin{pmatrix}-1&1&0\\-1&-1&0\\-1&0&1\end{pmatrix}$
*M*2 V1 *m*(*AC*)*I* $\frac{2}{m}$ *v*	$p^2 > b^2$, $b^2 > r^2 - q^2$			 *A*: $c^2 > b^2 > f^2 - a^2$	 *C*: $a^2 > b^2 > f^2 - c^2$	 *I*: $f^2 > b^2 > c^2 - a^2$	$\begin{pmatrix}0&1&-1\\1&1&0\\1&0&-1\end{pmatrix}$
*M*3 V2 *m*(*AC*)*I* $\frac{2}{m}$ *s*	$r^2 - q^2 > b^2$			 *A*: $f^2 - a^2 > b^2$	 *C*: $f^2 - c^2 > b^2$	 *I*: $c^2 - a^2 > b^2$	$\begin{pmatrix}-1&0&1\\-1&1&0\\-2&0&0\end{pmatrix}$
*M*4 V4 *m*(*AC*)*I* $\frac{2}{m}$ s^2	$b^2 = p^2$			 *A*: $b^2 = c^2$	 *C*: $b^2 = a^2$	 *I*: $b^2 = f^2$	$\begin{pmatrix}0&1&-1\\1&1&0\\1&0&-1\end{pmatrix}$
							$\begin{pmatrix}-1&1&0\\-1&-1&0\\-1&0&1\end{pmatrix}$

Table 3.1.2.3 (continued)

Delaunay–Voronoi type	Metric conditions	Selling tetrahedron	Projections along symmetry directions	Dirichlet domain in the unit cell	Transformation to the conventional cell
*M*5 V3 *m*(*AC*)*I* $\frac{2}{m}$ *v*	$b^2 = r^2 - q^2$			 *A*: $b^2 = f^2 - a^2$  *C*: $b^2 = f^2 - c^2$  *I*: $b^2 = c^2 - a^2$	$\begin{pmatrix} -1 & 0 & 1 \\ -1 & 1 & 0 \\ -2 & 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 1 & 0 & -1 \\ 1 & -1 & 0 \\ 0 & -1 & -1 \end{pmatrix}$
*M*6 V4 *mP* $\frac{2}{m}$ *s*	–				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
*T*1 V1 *aP* 1	–				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
*T*2 V2 *aP* 1	$\mathbf{a} \cdot \mathbf{b} = 0$				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
*T*3 V3 *aP* 1	$\mathbf{a} \cdot \mathbf{b} = 0$ $(\mathbf{a} + \mathbf{b} + \mathbf{c}) \cdot \mathbf{c} = 0$				$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

In some cases, different Selling patterns are given for one '*Symmetrische Sorte*'. This procedure avoids a final reduction step (*cf.* Patterson & Love, 1957) and simplifies the computational treatment significantly. The number of '*Symmetrische Sorten*', and thus the number of transformations which have to be applied, is smaller than the number of lattice characters according to Niggli. Note that the introduction of reduced bases using shortest lattice vectors causes complications in more than three dimensions (*cf.* Schwarzenberger, 1980).

3.1.2.4. Example of Delaunay reduction and standardization of the basis

Let the basis $\mathbf{B} = (\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$ given by the scalar products

$$\begin{pmatrix} g_{11} & g_{22} & g_{33} \\ g_{23} & g_{31} & g_{12} \end{pmatrix} = \begin{pmatrix} 6 & 8 & 8 \\ 4 & 2 & 3 \end{pmatrix}$$

or by $b_1 = 2.449$ ($\sqrt{6}$), $b_2 = b_3 = 2.828$ ($\sqrt{8}$) (in arbitrary units), $\beta_{23} = 60°$ ($\cos\beta_{23} = \frac{1}{2}$), $\beta_{13} = 73.22°$ ($\cos\beta_{13} = \sqrt{3}/6$), $\beta_{12} = 64.34°$ ($\cos\beta_{12} = \sqrt{3}/4$).

The aim is to find a standardized basis of shortest lattice vectors using Delaunay reduction. This example, given by B. Gruber (*cf.* Burzlaff & Zimmermann, 1985), shows the standardization problems remaining after the reduction.

The general reduction step can be described using Selling four flats. The corners are designated by the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d} = -\mathbf{a} - \mathbf{b} - \mathbf{c}$. The edges are marked by the scalar products among these vectors. If positive scalar products can be found, choose the largest: $\mathbf{a} \cdot \mathbf{b}$ (indicated as **ab** in Fig. 3.1.2.2*a*). The reduction transformation is: $\mathbf{a}_D = \mathbf{a}$, $\mathbf{b}_D = -\mathbf{b}$, $\mathbf{c}_D = \mathbf{c} + \mathbf{b}$, $\mathbf{d}_D = \mathbf{d} + \mathbf{b}$ (see Fig. 3.1.2.2*a*). In this example, this results in the Selling four flat shown in Fig. 3.1.2.2(*b*). The next step, shown in Fig. 3.1.2.2(*c*), uses the (maximal) positive scalar product for further reduction. Finally, using $\mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4 = -\mathbf{b}_1$ we get the result shown in Fig. 3.1.2.2(*d*).

The complete procedure can be expressed in a table, as shown in Table 3.1.2.4. Each pair of lines contains the starting basis and

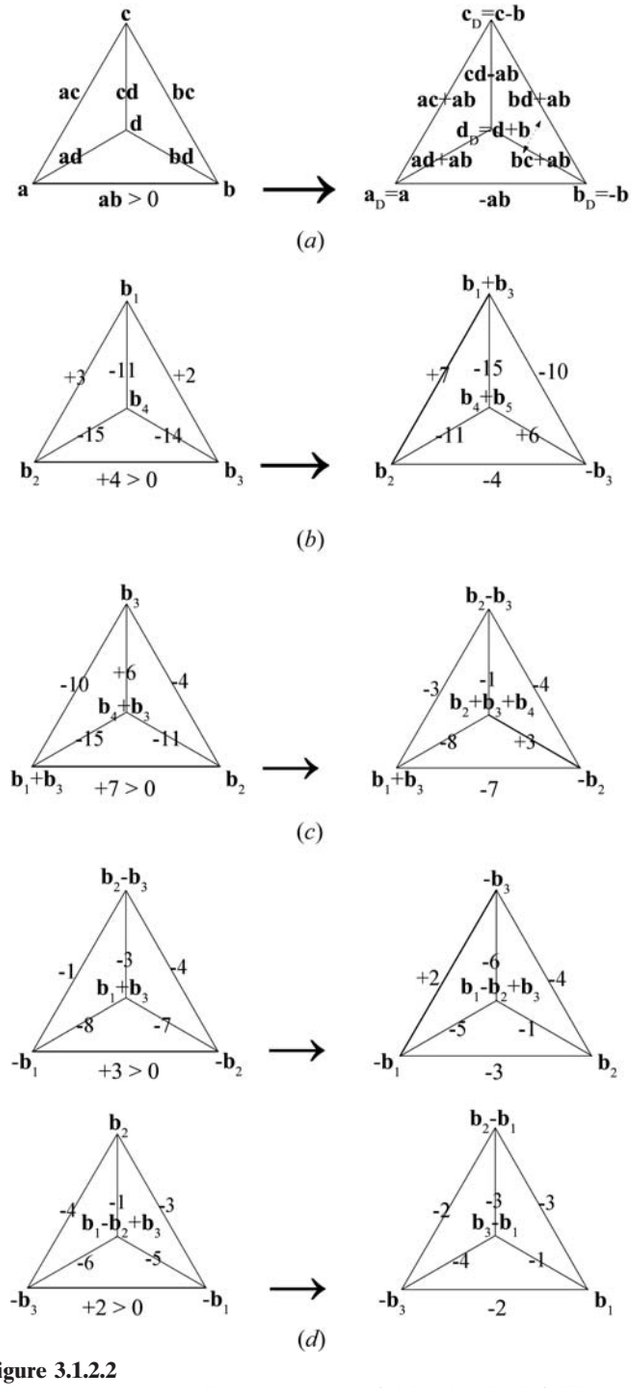


Figure 3.1.2.2
Delaunay reduction of Gruber's example (*cf.* Section 3.1.2.4). The edges of Selling tetrahedra are labelled by the scalar products of the vectors which designate the corners of the tetrahedra.

Table 3.1.2.5
Discussion of Gruber's example using the cell surface

No.	$(\mathbf{b}_1^s, \mathbf{b}_2^s, \mathbf{b}_3^s)$	Homogenous corner	Surface (surface units)
1	$(+\mathbf{b}_D, +\mathbf{a}_D, +\mathbf{c}_D)$	Non-acute	41.25
2	$(+\mathbf{b}_D, +\mathbf{a}_D, +\mathbf{d}_D)$	Non-acute	40.83
3	$(+\mathbf{b}_D, -\mathbf{a}_D, \mathbf{b}_D + \mathbf{c}_D)$	Acute	39.61
4	$(+\mathbf{b}_D, +\mathbf{c}_D, +\mathbf{d}_D)$	Non-acute	41.03
5	$(+\mathbf{b}_D, -\mathbf{d}_D, \mathbf{b}_D + \mathbf{c}_D)$	Acute	40.06

its scalar products before transformation as the first line, and then the transformed scalar products and the Delaunay basis after transformation below. In our case, four transformation steps are necessary. The result is

$$\mathbf{a}_D = -\mathbf{b}_3, \quad \mathbf{b}_D = \mathbf{b}_1, \quad \mathbf{c}_D = \mathbf{b}_2 - \mathbf{b}_1, \quad \mathbf{d}_D = \mathbf{b}_3 - \mathbf{b}_1.$$

The final Selling tetrahedron shows that the Dirichlet domain belongs to Voronoi type 1. It fulfils no symmetry condition and thus corresponds to an anorthic (triclinic) lattice.

For further standardization we consider the Delaunay set

$$\{\pm\mathbf{a}_D, \pm\mathbf{b}_D, \pm\mathbf{c}_D, \pm\mathbf{d}_D = -(\mathbf{a}_D + \mathbf{b}_D + \mathbf{c}_D), \pm(\mathbf{b}_D + \mathbf{c}_D), \pm(\mathbf{a}_D + \mathbf{c}_D), \pm(\mathbf{a}_D + \mathbf{b}_D)\}.$$

All bases of shortest lattice vectors $(\mathbf{b}_1^s, \mathbf{b}_2^s, \mathbf{b}_3^s)$ can be found:

$$|\mathbf{a}_D|^2 = 8, \quad |\mathbf{b}_D|^2 = 6, \quad |\mathbf{c}_D|^2 = 8, \quad |\mathbf{d}_D|^2 = 8,$$
$$|\mathbf{b}_D + \mathbf{c}_D|^2 = 8, \quad |\mathbf{a}_D + \mathbf{c}_D|^2 = 12, \quad |\mathbf{a}_D + \mathbf{b}_D|^2 = 10.$$

Any basis of shortest lattice vectors contains $\mathbf{b}_1^s = \mathbf{b}_D = \mathbf{b}_1$. For $\mathbf{b}_2^s$ the vectors $\mathbf{a}_D = -\mathbf{b}_3$, $\mathbf{c}_D = \mathbf{b}_2 - \mathbf{b}_1$, $\mathbf{d}_D = \mathbf{b}_3 - \mathbf{b}_1$ and $(\mathbf{b}_D + \mathbf{c}_D) = \mathbf{b}_2$ are possible. $\mathbf{b}_3^s$ can only be chosen from these vectors such that a linear independent triplet results.

The resulting five choices are given in Table 3.1.2.5. Any case corresponds to eight combinations of signs for the three basis vectors. The principle of the 'homogenous corner' (*i.e.*, there is always a pair of opposite corners of the corresponding cell where all angles are either non-acute or all three are acute) selects one of the bases in each case, thus five different bases remain. For the final choice the surfaces of the corresponding cells are given.

The maximal surface has cell No. 1 with the metrical parameters

$a = 2.449, b = c = 2.828$ Å, $\alpha = 104.47, \beta = 115.66, \gamma = 106.78°$.

A last possibility for the standardization is the interchange of **b** and **c** with inversion of all basis vectors. In this way the sequence of β and γ can be interchanged:

$a = 2.449, b = c = 2.828$ Å, $\alpha = 104.47, \beta = 106.78, \gamma = 115.66°$.

Table 3.1.2.4
Delaunay reduction for Gruber's example

a	**b**	**c**	**d**	**ab**, $\mathbf{a}_D\mathbf{b}_D$	**ac**, $\mathbf{a}_D\mathbf{c}_D$	**ad**, $\mathbf{a}_D\mathbf{d}_D$	**bc**, $\mathbf{b}_D\mathbf{c}_D$	**bd**, $\mathbf{b}_D\mathbf{d}_D$	**cd**, $\mathbf{c}_D\mathbf{d}_D$	$\mathbf{a}_D$	$\mathbf{b}_D$	$\mathbf{c}_D$	$\mathbf{d}_D$
$\mathbf{b}_2$	$\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_4$	+4 −4	+3 +7	−15 −11	+2 −10	14 +6	−11 −15	$\mathbf{b}_2$	$-\mathbf{b}_3$	$\mathbf{b}_1 + \mathbf{b}_3$	$\mathbf{b}_4 + \mathbf{b}_3$
$\mathbf{b}_1 + \mathbf{b}_3$	$\mathbf{b}_2$	$-\mathbf{b}_3$	$\mathbf{b}_3 + \mathbf{b}_4$	+7 −7	−10 −3	−15 −8	−4 −4	−11 +3	+6 −1	$\mathbf{b}_1 + \mathbf{b}_3$	$-\mathbf{b}_2$	$\mathbf{b}_2 - \mathbf{b}_3$	$\mathbf{b}_2 + \mathbf{b}_3 + \mathbf{b}_4$
$-\mathbf{b}_1$	$-\mathbf{b}_2$	$\mathbf{b}_2 - \mathbf{b}_3$	$\mathbf{b}_1 + \mathbf{b}_3$	+3 −3	−1 +2	−8 −5	−4 −4	−7 −1	−3 −6	$-\mathbf{b}_1$	$\mathbf{b}_2$	$-\mathbf{b}_3$	$\mathbf{b}_1 - \mathbf{b}_2 + \mathbf{b}_3$
$-\mathbf{b}_3$	$-\mathbf{b}_1$	$\mathbf{b}_2$	$\mathbf{b}_1 - \mathbf{b}_2 + \mathbf{b}_3$	+2 −2	−4 −2	−6 −4	−3 −3	−5 −1	−1 −3	$-\mathbf{b}_3$	$\mathbf{b}_1$	$\mathbf{b}_2 - \mathbf{b}_1$	$\mathbf{b}_3 - \mathbf{b}_1$

3.1.3. Reduced bases

BY P. M. DE WOLFF

3.1.3.1. Introduction

Unit cells are usually chosen according to the conventions mentioned in Section 3.1.1, so one might think that there is no need for another standard choice. This is not true, however; conventions based on symmetry do not always permit unambiguous choice of the unit cell, and unconventional descriptions of a lattice do occur. They are often chosen for good reasons or they may arise from experimental limitations such as may occur, for example, in high-pressure work. So there is a need for normalized descriptions of crystal lattices.

Accordingly, the *reduced basis*[1] (Eisenstein, 1851; Niggli, 1928), which is a primitive basis unique (apart from orientation) for any given lattice, is at present widely used as a means of classifying and identifying crystalline materials. A comprehensive survey of the principles, the techniques and the scope of such applications is given by Mighell (1976). The present contribution merely aims at an exposition of the basic concepts and a brief account of some applications.

The main criterion for the reduced basis is a metric one: choice of the shortest three non-coplanar lattice vectors as basis vectors. Therefore, the resulting bases are, in general, widely different from any symmetry-controlled basis, *cf.* Section 3.1.1.

3.1.3.2. Definition

A primitive basis **a**, **b**, **c** is called a 'reduced basis' if it is right-handed and if the components of the metric tensor $\boldsymbol{G}$ (*cf.* Section 3.1.1)

$$\begin{matrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{c}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} \end{matrix} \qquad (3.1.3.1)$$

satisfy the conditions shown below. The matrix (3.1.3.1) for the reduced basis is called the *reduced form*.

Because of lattice symmetry there can be two or more possible orientations of the reduced basis in a given lattice but, apart from orientation, the reduced basis is unique.

Any basis, reduced or not, determines a unit cell – that is, the parallelepiped of which the basis vectors are edges. In order to test whether a given basis is the reduced one, it is convenient first to find the 'type' of the corresponding unit cell. The type of a cell depends on the sign of

$$T = (\mathbf{a}\cdot\mathbf{b})(\mathbf{b}\cdot\mathbf{c})(\mathbf{c}\cdot\mathbf{a}).$$

If $T > 0$, the cell is of type I, if $T \leq 0$ it is of type II. 'Type' is a property of the cell since T keeps its value when **a**, **b** or **c** is inverted. Geometrically speaking, such an inversion corresponds to moving the origin of the basis towards another corner of the cell. Corners with all three angles acute occur for cells of type I (one opposite pair, the remaining six corners having one acute and two obtuse angles). The other alternative, specified by main condition (ii) of Section 3.1.3.3, *viz* all three angles non-acute, occurs for cells of type II (one or more opposite pairs, the remaining corners having either one or two acute angles).

The conditions can all be stated analytically in terms of the components (3.1.3.1), as follows:

(*a*) Type-I cell

Main conditions:

$$\mathbf{a}\cdot\mathbf{a} \leq \mathbf{b}\cdot\mathbf{b} \leq \mathbf{c}\cdot\mathbf{c}; \quad |\mathbf{b}\cdot\mathbf{c}| \leq \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b}; \quad |\mathbf{a}\cdot\mathbf{c}| \leq \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}; \quad |\mathbf{a}\cdot\mathbf{b}| \leq \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \qquad (3.1.3.2a)$$

$$\mathbf{b}\cdot\mathbf{c} > 0; \quad \mathbf{a}\cdot\mathbf{c} > 0; \quad \mathbf{a}\cdot\mathbf{b} > 0. \qquad (3.1.3.2b)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{b}\cdot\mathbf{c} \leq \mathbf{a}\cdot\mathbf{c} \qquad (3.1.3.3a)$$

$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } \mathbf{a}\cdot\mathbf{c} \leq \mathbf{a}\cdot\mathbf{b} \qquad (3.1.3.3b)$$

$$\text{if } \mathbf{b}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} \leq 2\mathbf{a}\cdot\mathbf{c} \qquad (3.1.3.3c)$$

$$\text{if } \mathbf{a}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} \leq 2\mathbf{b}\cdot\mathbf{c} \qquad (3.1.3.3d)$$

$$\text{if } \mathbf{a}\cdot\mathbf{b} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} \leq 2\mathbf{b}\cdot\mathbf{c}. \qquad (3.1.3.3e)$$

(*b*) Type-II cell

Main conditions:

$$\text{as (3.1.3.2}a\text{)} \qquad (3.1.3.4a)$$

$$(|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) \leq \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \qquad (3.1.3.4b)$$

$$\mathbf{b}\cdot\mathbf{c} \leq 0; \quad \mathbf{a}\cdot\mathbf{c} \leq 0; \quad \mathbf{a}\cdot\mathbf{b} \leq 0. \qquad (3.1.3.4c)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } |\mathbf{b}\cdot\mathbf{c}| \leq |\mathbf{a}\cdot\mathbf{c}| \qquad (3.1.3.5a)$$

$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } |\mathbf{a}\cdot\mathbf{c}| \leq |\mathbf{a}\cdot\mathbf{b}| \qquad (3.1.3.5b)$$

$$\text{if } |\mathbf{b}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (3.1.3.5c)$$

$$\text{if } |\mathbf{a}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (3.1.3.5d)$$

$$\text{if } |\mathbf{a}\cdot\mathbf{b}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} = 0 \qquad (3.1.3.5e)$$

$$\text{if } (|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) = \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \text{ then } \mathbf{a}\cdot\mathbf{a} \leq 2|\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|. \qquad (3.1.3.5f)$$

The geometrical interpretation in the following sections is given in order to make the above conditions more explicit rather than to replace them, since the analytical form is obviously the most suitable one for actual verification.

3.1.3.3. Main conditions

The main conditions[2] express the following two requirements:

(i) Of all lattice vectors, none is shorter than **a**; of those not directed along **a**, none is shorter than **b**; of those not lying in the **ab** plane, none is shorter than **c**. This requirement is expressed analytically by (3.1.3.2*a*), and for type-II cells by (3.1.3.4*b*), which for type-I cells is redundant.

(ii) The three angles between basis vectors are either all acute or all non-acute, conditions (3.1.3.2*b*) and (3.1.3.4*c*). As shown in Section 3.1.3.2 for a given unit cell, the origin corner can always be chosen so as to satisfy either the first alternative of this condition (if the cell is of type I) or the second (if the cell is of type II).

[1] Very often, the term 'reduced cell' is used to indicate this normalized lattice description. To avoid confusion, we shall use 'reduced basis', since it is actually a basis and some of the criteria are related precisely to the difference between unit cells and vector bases.

[2] In a book on reduced cells and on retrieval of symmetry information from lattice parameters, Gruber (1978) reformulated the main condition (i) as a minimum condition on the sum $s = a + b + c$. He also examined the surface areas of primitive unit cells in a given lattice, which are easily shown to be proportional to the corresponding sums $s^* = a^* + b^* + c^*$ for the reciprocal bases. He finds that if there are two or more non-congruent cells with minimum s ('Buerger cells'), these cells always have different values of s^*. Gruber (1989) proposes a new criterion to replace the conditions (3.1.3.2*a*)–(3.1.3.5*f*), *viz* that, among the cells with the minimum s value, the one with the smallest value of s^* be chosen (which need not be the absolute minimum of s^* since that may occur for cells that are not Buerger cells). The analytic form of this criterion is identical to (3.1.3.2*a*)–(3.1.3.5*e*); only (3.1.3.5*f*) is altered. For further details, see Section 3.1.4.

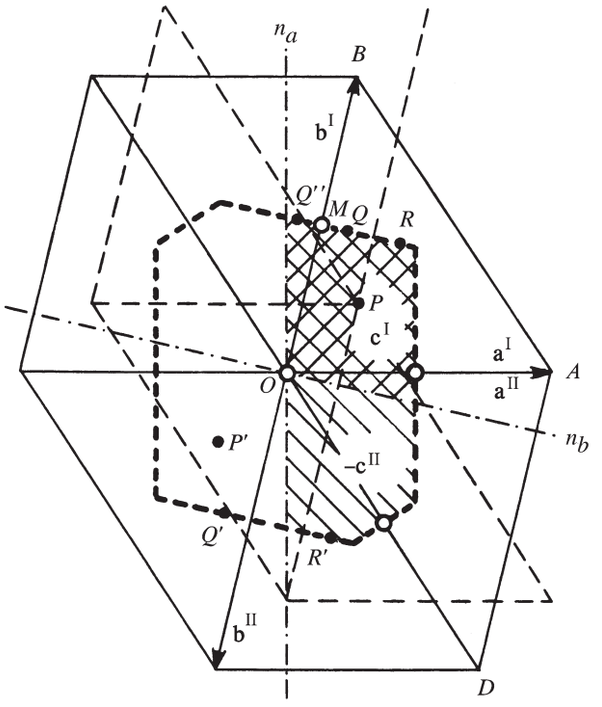


Figure 3.1.3.1
The net of lattice points in the plane of the reduced basis vectors **a** and **b**; *OBAD* is a primitive mesh. The actual choice of **a** and **b** depends on the position of the point *P*, which is the projection of the point P_0 in the next layer (supposed to lie above the paper, thin dashed lines) closest to *O*. Hence, *P* is confined to the Voronoi domain (dashed hexagon) around *O*. For a given interlayer distance, *P* defines the complete lattice. In that sense, *P* and *P*′ represent identical lattices; so do *Q*, *Q*′ and *Q*″, and also *R* and *R*′. When *P* lies in a region marked $-c^{II}$ (hatched), the reduced type-II basis is formed by $\mathbf{a}^{II}$, $\mathbf{b}^{II}$ and $\mathbf{c} = -\overrightarrow{OP}_0$. Regions marked c^I (cross-hatched) have the reduced type-I basis $\mathbf{a}^I$, $\mathbf{b}^I$ and $\mathbf{c} = +\overrightarrow{OP}_0$. Small circles in *O*, *M etc.* indicate twofold rotation points lying on the region borders (see text).

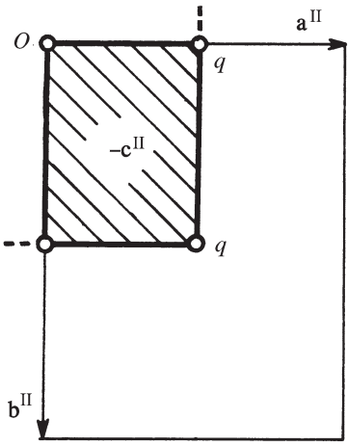


Figure 3.1.3.2
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I and type-II regions are marked as in Fig. 3.1.3.1. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net primitive orthogonal; special conditions (3.1.3.5*c*), (3.1.3.5*d*).

Condition (i) is by far the most essential one. It uniquely defines the lengths *a*, *b* and *c*, and limits the angles to the range $60 \leq \alpha, \beta, \gamma \leq 120°$. However, there are often different unit cells satisfying (i), *cf.* Gruber (1973). In order to find the reduced basis, starting from an arbitrary one given by its matrix (3.1.3.1), one can: (*a*) find some basis satisfying (i) and (ii) and if necessary modify it so as to fulfil the special conditions as well; (*b*) find all bases satisfying (i) and (ii) and test them one by one with regard to the special conditions until the reduced form is found. Method (*a*) relies mainly on an algorithm by Buerger (1957, 1960), *cf.* also Mighell (1976). Method (*b*) stems from a theorem and an algorithm, both derived by Delaunay (1933); the theorem states that the desired basis vectors **a**, **b** and **c** are among seven (or fewer) vectors – the distance vectors between parallel faces of the Voronoi domain – which follow directly from the algorithm. The method has been established and an example is given by Delaunay *et al.* (1973), *cf.* Section 3.1.2.3 where this method is described.

3.1.3.4. Special conditions

For a given lattice, the main condition (i) defines not only the lengths *a*, *b*, *c* of the reduced basis vectors but also the plane containing **a** and **b**, in the sense that departures from special conditions can be repaired by transformations which do not change this plane. An exception can occur when $b = c$; then such transformations must be supplemented by interchange(s) of **b** and **c** whenever either (3.1.3.3*b*) or (3.1.3.5*b*) is not fulfilled. All the other conditions can be conveniently illustrated by projections of part of the lattice onto the **ab** plane as shown in Figs. 3.1.3.1 to 3.1.3.5. Let us represent the vector lattice by a point lattice. In Fig. 3.1.3.1, the net in the **ab** plane (of which *OBAD* is a primitive mesh; $OA = a$, $OB = b$) is shown as well as the projection (normal to that plane) of the adjoining layer which is assumed to lie above the paper. In general, just one lattice node P_0 of that layer, projected in Fig. 3.1.3.1 as *P*, will be closer to the origin than all others. Then the vector $\overrightarrow{OP}_0$ is $\pm\mathbf{c}$ according to condition (i). It should be stressed that, though the **ab** plane is most often (see above) correctly established by (i), the vectors **a**, **b** and **c** still have to be chosen so as to comply with (ii), with the special conditions, and with right-handedness. The result will depend on the position of *P* with respect to the net. This dependence will now be investigated.

The inner hexagon shown, which is the two-dimensional Voronoi domain around *O*, limits the possible projected positions *P* of P_0. Its short edges, normal to *OD*, result from (3.1.3.4*b*); the other edges from (3.1.3.2*a*). If the spacing *d* between **ab** net planes is smaller than *b*, the region allowed for *P* is moreover limited inwardly by the circle around *O* with radius $(b^2 - d^2)^{1/2}$, corresponding to the projection of points P_0 for which $OP_0 = c = b$. The case $c = b$ has been dealt with, so in order to simplify the drawings we shall assume $d > b$. Then, for a given value of *d*, each point within the above-mentioned hexagonal domain, regarded as the projection of a lattice node P_0 in the next layer, completely defines a lattice based on $\overrightarrow{OA}$, $\overrightarrow{OB}$ and $\overrightarrow{OP}_0$. Diametrically opposite points like *P* and *P*′ represent the same lattice in two orientations differing by a rotation of 180° in the plane of the figure. Therefore, the systematics of reduced bases can be shown completely in just half the domain. As a halving line, the n_a normal to *OA* is chosen. This is an important boundary in view of condition (ii), since it separates points *P* for which the angle between OP_0 and *OA* is acute from those for which it is obtuse.

Similarly, n_b, normal to *OB*, separates the sharp and obtuse values of the angles P_0OB. It follows that if *P* lies in the obtuse sector (cross-hatched area) between n_a and n_b, the reduced cell is

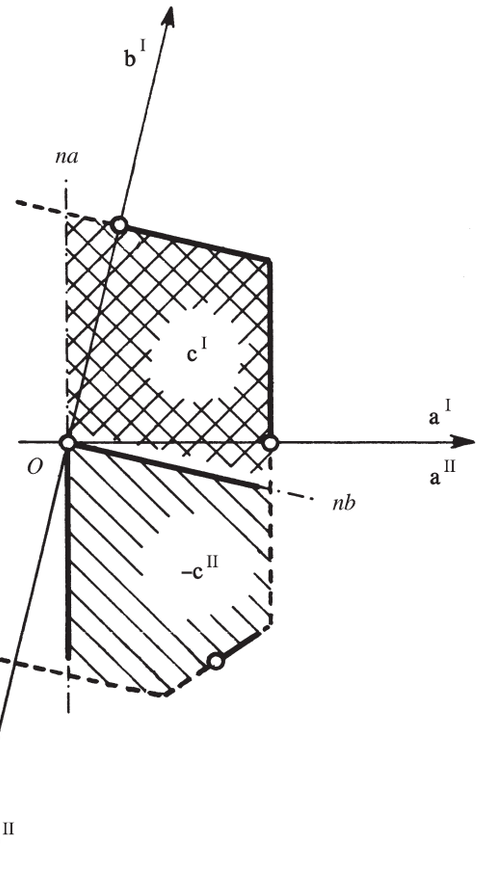


Figure 3.1.3.3
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net oblique; special conditions (3.1.3.3*c*), (3.1.3.3*d*), (3.1.3.5*f*).

of type I, with basis vectors $\mathbf{a}^{\rm I}$, $\mathbf{b}^{\rm I}$, and $OP_0 = +\mathbf{c}$. Otherwise (hatched area), we have a type-II reduced cell, with $OP_0 = -\mathbf{c}$ and $+\mathbf{a}$ and $+\mathbf{b}$ as shown by $\mathbf{a}^{\rm II}$ and $\mathbf{b}^{\rm II}$.

Since type II includes the case of right angles, the borders of this region on n_a and n_b are inclusive. Other borderline cases are points like R and R', separated by **b** and thus describing the same lattice. By condition (3.1.3.5*c*) the reduced cell for such cases is excluded from type II (except for rectangular **a**, **b** nets, *cf.* Fig. 3.1.3.2); so the projection of **c** points to R, not R'. Accordingly, this part of the border is inclusive for the type-I region and exclusive (at R') for the type-II region as indicated in Fig. 3.1.3.3. Similarly, (3.1.3.5*d*) defines which part of the border normal to OA is inclusive.

The inclusive border is seen to end where it crosses OA, OB or OD. This is prescribed by the conditions (3.1.3.3*d*), (3.1.3.3*c*) and (3.1.3.5*f*), respectively. The explanation is given in Fig. 3.1.3.1 for (3.1.3.3*c*): The points Q and Q'' represent the same lattice because Q' (diametrically equivalent to Q as shown before) is separated from Q'' by the vector **b**. Hence, the point M halfway between O and B is a twofold rotation point just like O. For a primitive orthogonal **a**, **b** net, only type II occurs according to (3.1.3.5*c*) and (3.1.3.5*d*), *cf.* Fig. 3.1.3.2. A centred orthogonal **a**, **b** net of elongated character (shortest net vector in a symmetry direction, *cf.* Section 3.1.3.5) is depicted in Fig. 3.1.3.4. It yields type-I cells except when $\beta = 90°$ [condition (3.1.3.5*c*)]. Moreover, (3.1.3.3*c*) eliminates part of the type-I region as compared to Fig.

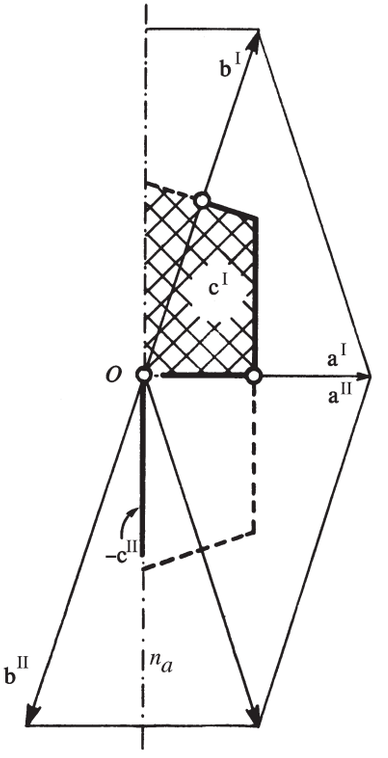


Figure 3.1.3.4
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I region is cross-hatched; the type-II region is a mere line. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net centred orthogonal (elongated); special conditions (3.1.3.3*e*), (3.1.3.5*e*).

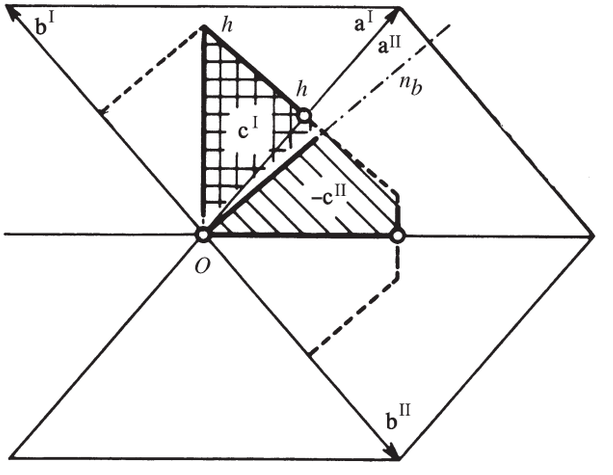


Figure 3.1.3.5
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. Type-I and type-II regions are marked as in Fig. 3.1.3.1. n_b belongs to the type-II region. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net centred orthogonal (compressed); special conditions (3.1.3.3*a*), (3.1.3.5*a*).

3.1.3.3. Finally, a centred net with compressed character (shortest two net vectors equal in length) requires criteria allowing unambiguous designation of **a** and **b**. These are conditions (3.1.3.3*a*) and (3.1.3.5*a*), *cf.* Fig. 3.1.3.5. The simplicity of these bisecting conditions, similar to those for the case $b = c$ mentioned initially, is apparent from that figure when compared

Table 3.1.3.1
The parameters $D = \mathbf{b}\cdot\mathbf{c}$, $E = \mathbf{a}\cdot\mathbf{c}$ and $F = \mathbf{a}\cdot\mathbf{b}$ of the 44 lattice characters ($A = \mathbf{a}\cdot\mathbf{a}$, $B = \mathbf{b}\cdot\mathbf{b}$, $C = \mathbf{c}\cdot\mathbf{c}$)

The character of a lattice given by its reduced form (3.1.3.1) is the first one that agrees when the 44 entries are compared with that reduced form in the sequence given below (suggested by Gruber). Such a logical order is not always obeyed by the widely used character numbers (first column), which therefore show some reversals, *e.g.* 4 and 5.

No.	Type	D	E	F	Lattice symmetry	Bravais type of lattice†	Transformation to a conventional basis (*cf.* footnote ‡ to Table 3.1.3.2)
$A = B = C$							
1	I	$A/2$	$A/2$	$A/2$	Cubic	*cF*	$1\bar{1}1/11\bar{1}/\bar{1}11$
2	I	D	D	D	Rhombohedral	*hR*	$1\bar{1}0/101/\bar{1}\bar{1}\bar{1}$
3	II	0	0	0	Cubic	*cP*	100/010/001
5	II	$-A/3$	$-A/3$	$-A/3$	Cubic	*cI*	101/110/011
4	II	D	D	D	Rhombohedral	*hR*	$1\bar{1}0/\bar{1}01/\bar{1}\bar{1}\bar{1}$
6	II	D‡	D	F	Tetragonal	*tI*	011/101/110
7	II	D‡	E	E	Tetragonal	*tI*	101/110/011
8	II	D‡	E	F	Orthorhombic	*oI*	$\bar{1}\bar{1}0/\bar{1}01/0\bar{1}\bar{1}$
$A = B$, no conditions on C							
9	I	$A/2$	$A/2$	$A/2$	Rhombohedral	*hR*	$100/\bar{1}10/\bar{1}\bar{1}3$
10	I	D	D	F	Monoclinic	*mC*	$110/1\bar{1}0/00\bar{1}$
11	II	0	0	0	Tetragonal	*tP*	100/010/001
12	II	0	0	$-A/2$	Hexagonal	*hP*	100/010/001
13	II	0	0	F	Orthorhombic	*oC*	$110/\bar{1}10/001$
15	II	$-A/2$	$-A/2$	0	Tetragonal	*tI*	$\underline{1}00/0\underline{1}0/112$
16	II	D‡	D	F	Orthorhombic	*oF*	$\bar{1}\bar{1}0/\bar{1}10/112$
14	II	D	D	F	Monoclinic	*mC*	$110/\bar{1}10/001$
17	II	D‡	E	F	Monoclinic	*mC*	$1\bar{1}0/110/\bar{1}01$
$B = C$, no conditions on A							
18	I	$A/4$	$A/2$	$A/2$	Tetragonal	*tI*	$0\bar{1}1/1\bar{1}\bar{1}/100$
19	I	D	$A/2$	$A/2$	Orthorhombic	*oI*	$\bar{1}00/0\bar{1}1/\bar{1}11$
20	I	D	E	E	Monoclinic	*mC*	$011/01\bar{1}/100$
21	II	0	0	0	Tetragonal	*tP*	010/001/100
22	II	$-B/2$	0	0	Hexagonal	*hP*	010/001/100
23	II	D	0	0	Orthorhombic	*oC*	$011/0\bar{1}1/100$
24	II	D‡	$-A/3$	$-A/3$	Rhombohedral	*hR*	$121/0\bar{1}1/100$
25	II	D	E	E	Monoclinic	*mC*	$011/0\bar{1}1/100$
No conditions on A, B, C							
26	I	$A/4$	$A/2$	$A/2$	Orthorhombic	*oF*	$100/\bar{1}20/\bar{1}02$
27	I	D	$A/2$	$A/2$	Monoclinic	*mC*	$\bar{1}20/\bar{1}00/0\bar{1}1$
28	I	D	$A/2$	$2D$	Monoclinic	*mC*	$\bar{1}00/\bar{1}02/010$
29	I	D	$2D$	$A/2$	Monoclinic	*mC*	$100/1\bar{2}0/00\bar{1}$
30	I	$B/2$	E	$2E$	Monoclinic	*mC*	$010/012/\bar{1}00$
31	I	D	E	F	Triclinic	*aP*	100/010/001
32	II	0	0	0	Orthorhombic	*oP*	100/010/001
40	II	$-B/2$	0	0	Orthorhombic	*oC*	$0\bar{1}0/012/\bar{1}00$
35	II	D	0	0	Monoclinic	*mP*	$0\bar{1}0/\bar{1}00/00\bar{1}$
36	II	0	$-A/2$	0	Orthorhombic	*oC*	$100/\bar{1}02/010$
33	II	0	E	0	Monoclinic	*mP*	100/010/001
38	II	0	0	$-A/2$	Orthorhombic	*oC*	$\bar{1}00/120/00\bar{1}$
34	II	0	0	F	Monoclinic	*mP*	$\bar{1}00/00\bar{1}/0\bar{1}0$
42	II	$-B/2$	$-A/2$	0	Orthorhombic	*oI*	$\bar{1}00/0\bar{1}0/112$
41	II	$-B/2$	E	0	Monoclinic	*mC*	$0\bar{1}2/0\bar{1}0/\bar{1}00$
37	II	D	$-A/2$	0	Monoclinic	*mC*	$102/100/010$
39	II	D	0	$-A/2$	Monoclinic	*mC*	$\bar{1}20/\bar{1}00/00\bar{1}$
43	II	D§	E	F	Monoclinic	*mI*	$\bar{1}00/\bar{1}\bar{1}2/0\bar{1}0$
44	II	D	E	F	Triclinic	*aP*	100/010/001

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). The capital letter of the symbols in this column indicates the centring type of the cell as obtained by the transformation in the last column. For this reason, the standard symbols *mS* and *oS* are not used here. ‡ $2|D + E + F| = A + B$. § $2|D + E + F| = A + B$ plus $|2D + F| = B$.

with Fig. 3.1.3.3. This compressed type of centred orthogonal **a**, **b** net is limited by the case of a hexagonal net (where it merges with the elongated type, Fig. 3.1.3.4) and by the centred quadratic net (where it merges with the primitive orthogonal net, Fig. 3.1.3.2). In the limit of the hexagonal net, the triangle *Ohh* in Figs. 3.1.3.4 and 3.1.3.5 is all that remains, it is of type I except for the point *O*. For the quadratic net, only the type-II region in Fig. 3.1.3.5, then a triangle with all edges inclusive, is left. It corresponds to the triangle *Oqq* in Fig. 3.1.3.2.

3.1.3.5. Lattice characters

Apart from being unique, the reduced cell has the further advantage of allowing a much finer differentiation between types of lattices than is given by the Bravais types. For two-dimensional lattices, this is apparent already in the last section where the centred orthogonal class is subdivided into nets with elongated character and those with compressed character, depending on whether the shortest net vector is, or is not, a symmetry direction.

Table 3.1.3.2
Lattice characters described by relations between conventional cell parameters

Under each of the roman numerals below 'Lattice characters in', *numbers* of characters (*cf.* Table 3.1.3.1, first column) are listed for which the key parameter p lies in the interval defined by the same roman numeral below 'Intervals of p'. For instance, a lattice with character No. 15 under IV has $p = c/a$; so it falls in the interval IV with $2^{1/2} < c/a$ ($< \infty$); No. 33 under II has $p = b$; therefore the interval $a - c$ for II yields the relation $a < b < c$.

Lattice symmetry	Bravais type of lattice†	p = key parameter	Lattice characters in I	II	III	IV	Intervals of p I	II	III	IV		Conventions‡
Tetragonal	*tP*	c/a	21	11	–	–	0	1	∞	–	–	
Tetragonal	*tI*	c/a	18	6	7	15	0	$(2/3)^{1/2}$	1	$2^{1/2}$	∞	
Hexagonal	*hP*	c/a	22	12	–	–	0	1	∞	–	–	
Rhombohedral	*hR*	c/a	24	4	2	9	0	$(3/8)^{1/2}$	$(3/2)^{1/2}$	$6^{1/2}$	∞	Hexagonal axes
Orthorhombic	*oP*	–	32 no relations				–	–	–	–	–	$a < b < c$
Orthorhombic	*oS*											
$b < a\sqrt{3}$		c	23	13	–	–	0	*d*§	∞	–	–	$a < b$
$b > a\sqrt{3}$		c	40	36	38	–	0	*a*	*d*§	∞	–	
Orthorhombic	*oI*	*r*¶	8	19	42	–	0	*a*	*b*	∞	–	$a < b < c$
Orthorhombic	*oF*	b/a	16	26	–	–	1	$3^{1/2}$	∞	–	–	$a < b < c$
Monoclinic	*mP*	b	35	33	34	–	0	*a*	*c*	∞	–	$a < c$††
Monoclinic	*mS*											
Centred net = 1‡‡		b/a	–	–	–	28 or 29						
Centred net = 2		b/a	–	–	–	30						
Centred net = 2, 3		b/a	37 or 41	20	25	–	0	$(1/3)^{1/2}$	1	$3^{1/2}$	∞	*C* centred††
Centred net = 1, 2, 3		b/a	27 or 39	10 or 17	14	–						
Centred net = 3		b/a	43	–	–	–	1	∞	–	–	–	*I* centred††
Triclinic	*aP*	α, β, γ	31	44	–	–	60°	90°	120°	–	–	$a < b < c$
Cubic	*cP*	–		3	no relations		–	–	–	–	–	
	cI	–		5			–	–	–	–	–	
	cF	–		1			–	–	–	–	–	

† The symbols for Bravais types of lattices were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985). ‡ These conventions refer to the cells obtained by the transformations of Table 3.1.3.1. They have been chosen for convenience in this table. § $d = \frac{1}{2}(a^2 + b^2)^{1/2}$. ¶ $r = \frac{1}{2}(a^2 + b^2 + c^2)^{1/2}$. †† Setting with unique axis b; $\beta > 90°$; $a < c$ for both *P* and *I* cells, $a < c$ or $a > c$ for *C* cells. ‡‡ This number specifies the centred net among the three orthogonal nets parallel to the twofold axis and passing through (1) the shortest, (2) the second shortest, and (3) the third shortest lattice vector perpendicular to the axis. For example, '2, 3' means that either net (2) or net (3) is the centred one.

It is impossible to perform a continuous deformation – within the centred orthogonal type – of an elongated net into a compressed one, since one has to pass through either a hexagonal or a quadratic net.

In three dimensions, lattices are of the same character if, first, a continuous deformation of one into the other is possible without leaving the Bravais type. Secondly, it is required that all matrix elements of the reduced form (3.1.3.1) change continuously during such a deformation. These criteria lead to 44 different *lattice characters* (Niggli, 1928; Buerger, 1957). Each of them can be recognized easily from the relations between the elements of the reduced form given in Table 3.1.3.1 [adapted from Table 5.1.3.1 in *International Tables for X-ray Crystallography* (1969), which was improved by Mighell & Rodgers (1980)]. The numbers in column 1 of this table are at the same time used as a general notation of the lattice characters themselves. We speak, for example, about the lattice character No. 7 (which is part of the Bravais type *tI*) *etc*.

In Table 3.1.3.2, another description of lattice characters is given by grouping together all characters of a given Bravais type and by indicating for each character the corresponding interval of values of a suitable parameter p, expressed in the usual parameters of a conventional cell. In systems where no generally accepted convention exists, the choice of this cell has been made for convenience in the last column of this table.

The subdistinctions 'centred net = 1, 2 or 3' for the monoclinic centred type are closely related to the description in other conventions. For instance, they correspond to *C*-, *A*- or *I*-centred cells, respectively, if **b** is the unique axis and **a** and **c** are the shortest vectors ($a < c$) perpendicular to **b**; note that in Table 3.1.3.2 only *C* and *I*, not *A*, cells are listed. From the multiple entries in Table 3.1.3.2 for this type, it follows that the description in terms of *b/a* is not exhaustive; the distinctions depend upon rather intricate relations (*cf.* Mighell *et al.*, 1975; Mighell & Rodgers, 1980).

No attempt has been made in Table 3.1.3.2 to specify whether the end points of p intervals are inclusive or not. For practical purposes, they can always be taken to be non-inclusive. Indeed, the end points correspond either to a different Bravais type or to a purely geometric singularity without physical significance. If p is very close to an interval limit of the latter kind, one should be aware of the fact that different measurements of such a lattice may yield different characters, with totally differing aspects of the reduced form.

3.1.3.6. Applications

Classification. The reduced basis can be used to derive the Bravais-lattice type and the conventional cell parameters, starting from an arbitrary description of the lattice. For this purpose, the reduced form is first derived from the given description, *e.g.* by means of the algorithm of Křivý & Gruber (1976). Subsequently it is compared with the reduced forms (Table 3.1.3.1) for the 44 lattice characters and transformed to the appropriate conventional cell. Thus the reduced cell is helpful as an accessory in classifications based on conventional cells.

Alternatively, the parameters of the reduced form itself (either of the direct lattice or of the reciprocal lattice) can be used as a basis for determinative classification.

Comparison of lattices. Two lattices, defined by their reduced cells, can be compared on a rigorous basis to find out whether they are identical lattices or are related by one cell being a subcell of the other (Santoro *et al.*, 1980).

Further properties of lattices are discussed in Section 3.1.4.

P. M. de Wolff wishes to thank Dr B. Gruber (Prague) and Dr A. Santoro (Washington) for reading the manuscript for Section 3.1.3 and for suggesting several improvements as well as pointing out errors, especially in Tables 3.1.3.1 and 3.1.3.2.

3.1.4. Further properties of lattices

By B. Gruber and H. Grimmer

3.1.4.1. Further kinds of reduced cells

In Section 3.1.3.2, a 'reduced basis' of a lattice is defined which permits a unique representation of this lattice. It was introduced into crystallography by Niggli (1928) and incorporated into *International Tables for X-ray Crystallography* (1969), Vol. I. Originating from algebra (Eisenstein, 1851), a reduced basis is defined in a rather complicated manner [conditions (3.1.3.2*a*) to (3.1.3.5*f*) in Section 3.1.3.2] and lacks any geometrical meaning. A cell spanned by a reduced basis is called the *Niggli cell*.

However, unique primitive cells may be introduced also in other ways that – unlike the Niggli cell[3] – have significant geometrical features based mainly on extremal principles (Gruber, 1989). We shall describe some of them below.

If a (primitive) cell of the lattice **L** fulfils the condition

$$a + b + c = \min$$

on the set of all primitive cells of **L**, we call it a *Buerger cell*. This cell need not be unique with regard to its shape in the lattice. There exist lattices with 1, 2, 3, 4 and 5 (but not more) Buerger cells differing in shape. The uniqueness can be achieved by various additional conditions. In this way, we can arrive at the following four reduced cells:

(i) the Buerger cell with minimum surface;[4]
(ii) the Buerger cell with maximum surface;
(iii) the Buerger cell with minimum deviation;[5]
(iv) the Buerger cell with maximum deviation.

Equivalent definitions can be obtained by replacing the term 'surface' in (i) and (ii) by the expression

$$\sin\alpha + \sin\beta + \sin\gamma$$

or

$$\sin\alpha \sin\beta \sin\gamma,$$

and by replacing the 'deviation' in (iii) and (iv) by

$$|\cos\alpha| + |\cos\beta| + |\cos\gamma|$$

or

$$|\cos\alpha \cos\beta \cos\gamma|.$$

A Buerger cell can agree with more than one of the definitions

$$\text{(i), (ii), (iii), (iv).} \qquad (3.1.4.1)$$

[3] See, however, later parts of this section.
[4] Meaning that this cell has the smallest surface of all Buerger cells of the lattice.
[5] The deviation of a cell is the number $|90^\circ - \alpha| + |90^\circ - \beta| + |90^\circ - \gamma|$.

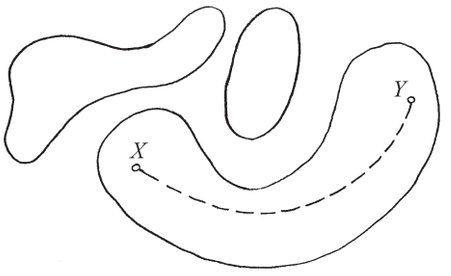


Figure 3.1.4.1
A set **M** in $\mathbb{E}^2$ consisting of three components.

For example, if a lattice has only one Buerger cell, then this cell agrees with all the definitions in (3.1.4.1). However, there exist also Buerger cells that are in agreement with none of them. Thus, the definitions (3.1.4.1) do not imply a partition of Buerger cells into classes.

It appears that case (iv) coincides with the Niggli cell. This is important because this cell can now be defined by a simple geometrical property instead of a complicated system of conditions.

Further reduced cells can be obtained by applying the definitions (3.1.4.1) to the reciprocal lattice. Then, to a Buerger cell in the reciprocal lattice, there corresponds a primitive cell with absolute minimum surface[6] in the direct lattice.

The reduced cells according to the definitions (3.1.4.1) can be recognized by means of a table and found in the lattice by means of algorithms. Detailed mutual relationships between them have been ascertained.

3.1.4.2. Topological characterization of lattice characters

In his thorough analysis of lattice characters, de Wolff (1988) remarks that so far they have not been defined as clearly as the Bravais types and that an exact general definition does not exist. Gruber (1992) tried to base such a definition on topological concepts.

The crucial notion is the decomposition of a set **M** of points of the n-dimensional Euclidean space $\mathbb{E}^n$ into equivalence classes called *components* of the set **M**. They can be defined as follows: Two points X, Y of the set **M** belong to the same component if they can be connected by a *continuous* path which lies entirely in the set **M** (Fig. 3.1.4.1). This partition of the set **M** into components is unique and is determined solely by the set **M**.

Now let us return to lattices. To any lattice **L** there is attached a point in $\mathbb{E}^5$ called the *Niggli point* of **L**. It is the point

$$\left[\frac{\mathbf{a}\cdot\mathbf{a}}{\mathbf{c}\cdot\mathbf{c}}, \frac{\mathbf{b}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{b}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}\right] \qquad (3.1.4.2)$$

provided that the vectors **a**, **b**, **c** describe the Niggli cell of **L** and fulfil the conditions (3.1.3.2*a*) to (3.1.3.5*f*) of Section 3.1.3.2. If $\mathscr{L}$ is a set of lattices then the set of Niggli points of all lattices of $\mathscr{L}$ is called the *Niggli image* of $\mathscr{L}$.

Thus we can speak about the Niggli image of a Bravais type $\mathscr{T}$. This Niggli image is a part of $\mathbb{E}^5$ and so can be partitioned into components. This division of Niggli points induces back a division of lattices of the Bravais type $\mathscr{T}$. It turns out that this division is identical with the division of $\mathscr{T}$ into lattice characters as introduced in Section 3.1.3.5. This fact, used conversely, can be considered an exact definition of the lattice characters: Two lattices of Bravais type $\mathscr{T}$ are said to be of the same lattice

[6] This cell need not be a Buerger cell.

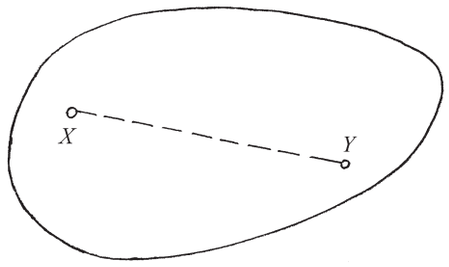


Figure 3.1.4.2
A convex set in $\mathbb{E}^2$.

character if their Niggli points lie in the same component of the Niggli image of $\mathscr{T}$.

We can, of course, also speak about Niggli images of particular lattice characters. According to their definition, these images are connected sets. However, much more can be stated about them: these sets are even *convex* (Fig. 3.1.4.2). This means that any two points of the Niggli image of a lattice character can be connected by a *straight segment* lying totally in this Niggli image. From this property, it follows that the lattice characters may be defined also in the following equivalent way:

We say that two lattices of the same Bravais type belong to the same lattice character if one of them can be deformed into the other in such a way that the Niggli point of the deformed lattice moves *linearly* from the initial to the final position while the Bravais type of the lattice remains unchanged.

Unlike convexity, nothing can be said about whether the Niggli images of lattice characters are *open* sets (with regard to their dimension) or not. Both cases occur.

The lattice character of a lattice **L** can also be recognized [instead of by means of Table 3.1.3.1 or by Tables 1 and 3 in Gruber (1992)] by perpendicular projection of the **c** vector onto the **ab** plane provided the vectors **a**, **b**, **c** describe the Niggli cell of **L** and fulfil the conditions (3.1.3.2*a*) to (3.1.3.5*f*) in Section 3.1.3.2 (de Wolff & Gruber, 1991). See also Figs. 3.1.3.1 to 3.1.3.5.

3.1.4.3. A finer division of lattices

The 44 lattice characters form a subdivision of the 14 Bravais types. There is another commonly known subdivision of the Bravais types, namely the 24 Delaunay sorts (*Symmetrische Sorten*) (Delaunay, 1933; *International Tables for X-ray Crystallography*, 1952, Vol. I; *cf.* Section 3.1.2.3). However, the two divisions, being based on quite different principles, are incompatible: the 44 lattice characters do not form a subdivision of the 24 Delaunay sorts.

A natural problem arises to construct a division of lattices which would be a subdivision of both the lattice characters and the Delaunay sorts. However, we do not admit a purely mechanical intersection of both these divisions; we insist that their common subdivision be crystallographically meaningful.

Such a division was proposed by Gruber (1997*a*). It uses the fact that the Niggli points of all lattices lie in two five-dimensional polyhedra, say Ω^+ and Ω^-. The underlying idea, originating from H. Wondratschek, is based on the distribution of Niggli points among the vertices, edges, faces, three- and four-dimensional hyperfaces, and the interior of Ω^+ and Ω^-. This leads to a natural division of Niggli points and further to a division of lattices. This division has 67 classes, but is not suitable for crystallography because it does not constitute a subdivision of the Bravais types.

A modification of the idea is necessary. It consists of representing a lattice **L** by several points (instead of by one Niggli point) and the addition of two minor conditions. One of them concerns the diagonals of the Niggli cell and the other the bases of **L** which describe the Niggli cell.

Though these conditions are of little importance in themselves, they lead to a very useful notion, *viz* the division of all lattices into 127 classes which is a subdivision of both the lattice characters and the Delaunay sorts. The equivalence classes of this division are called *genera*. They form, in a certain sense, building blocks of both lattice characters and Delaunay sorts and show their mutual relationship.

The distribution of genera along the Bravais types is the following (the number of genera is given in parentheses): *cP* (1), *cI* (1), *cF* (1), *tP* (2), *tI* (5), *oP* (1), *oC* (8), *oI* (7), *oF* (3), *hP* (3), *hR* (4), *mP* (5), *mC* (43), *aP* (43). Thus, genera seem to be especially suitable for a finer classification of lattices of low symmetry.

The genus of a given lattice **L** can be determined – provided that the Niggli point of **L** is known – by means of a table containing explicit descriptions of all genera. These descriptions are formed by open linear systems of inequalities. Consequently, the ranges of conventional parameters of genera are open unlike those concerning the lattice characters.

Genera are denoted by symbols derived from the geometrical shape of Ω^+ and Ω^-. They can be visualized in the three-dimensional cross sections of these bodies. This gives a fairly good illustration of the relationships between genera.

However, the most important feature of genera seems to be the fact that lattices of the same genus agree in a surprisingly great number of crystallographically significant properties, such as the number of Buerger cells, the densest directions and planes, the symmetry of these planes *etc.* Even the formulae for the conventional cells are the same. The genus appears to be a remarkably strong bond between lattices.

3.1.4.4. Conventional cells

Conventional cells are dealt with in Section 3.1.1. They are illustrated in Fig. 3.1.2.1 and described in Table 3.1.2.2. This description, however, is not exhaustive enough for determining the Bravais type. In mathematical terms, the conditions in Table 3.1.2.2 are necessary but not sufficient. For example, the *C*-centred cell with

$$a = 6, \quad b = 8, \quad c = 5, \quad \cos\beta = -7/15, \quad \alpha = \gamma = 90^\circ \tag{3.1.4.3}$$

has the typical shape of a conventional cell of an *mC* lattice. But the lattice generated by the *C*-centred cell (3.1.4.3) is actually *hR* with the conventional rhombohedral basis vectors

$$\mathbf{c}, \quad (\mathbf{a}+\mathbf{b})/2, \quad (\mathbf{a}-\mathbf{b})/2.$$

It is a natural goal to establish a system of conditions for the conventional cells which would be not only necessary but also sufficient. This is done in Table 3.1.4.1. In order to make the conditions as simple as possible, the usual *mC* description of the monoclinic centred lattices is replaced by the *mI* description. The relation between the two descriptions is simple:

$$\mathbf{a}_I = -\mathbf{c}_C, \quad \mathbf{b}_I = \mathbf{b}_C, \quad \mathbf{c}_I = \mathbf{a}_C + \mathbf{c}_C.$$

The exact meaning of Table 3.1.4.1 is as follows: Suppose that a Bravais type different from *aP* is given and that its symbol appears in column 1 in the *i*th entry of Table 3.1.4.1. Then a lattice **L** is of this Bravais type if and only if there exists a cell (**a**, **b**, **c**) in **L** such that

Table 3.1.4.1
Conventional cells for the three-dimensional Bravais types of lattices and their limiting cases

All remaining lattices are covered by the anorthic (triclinic) Bravais type *aP*.

Bravais type of lattice	Centring mode of the cell (**a**, **b**, **c**)	Conditions	Limiting cases	Conventional basis (**a**′, **b**′, **c**′) for limiting case
cP	*P*	$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$		
cI	*I*	$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$		
cF	*F*	$a = b = c$, $\alpha = \beta = \gamma = 90^\circ$		
tP	*P*	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	$b = c \rightarrow cP$	**a**, **b**, **c**
tI	*I*	$c/\sqrt{2} \neq a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$	$c/\sqrt{2} = a \rightarrow cF$ $b = c \rightarrow cI$	**a** + **b**, **b** − **a**, **c** **a**, **b**, **c**
oP	*P*	$a < b < c$,† $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tP$ $b = c \rightarrow tP$	**a**, **b**, **c** ($c'/a' > 1$) **b**, **c**, **a** ($c'/a' < 1$)
oI	*I*	$a < b < c$, $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tI$ $b = c \rightarrow tI$	**a**, **b**, **c** ($c'/a' > 1$) **b**, **c**, **a** ($c'/a' < 1$)
oF	*F*	$a < b < c$, $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tI$ $b = c \rightarrow tI$	(**a** + **b**)/2, (**b** − **a**)/2, **c** ($c'/a' > 1$) (**b** + **c**)/2, (**c** − **b**)/2, **a** ($c'/a' < 1$)
oC	*C*	$a < b \neq a\sqrt{3}$, $\alpha = \beta = \gamma = 90^\circ$	$a = b \rightarrow tP$ $b = a\sqrt{3} \rightarrow hP$	(**a** + **b**)/2, (**b** − **a**)/2, **c** **a**, (**b** − **a**)/2, **c**
hP	*P*	$a = b$ $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$		
hR	*P*	$a = b = c$, $\alpha = \beta = \gamma$ $\alpha \neq 60^\circ, \alpha \neq 90^\circ, \alpha \neq \omega$‡	$\alpha = 60^\circ \rightarrow cF$ $\alpha = 90^\circ \rightarrow cP$ $\alpha = \omega \rightarrow cI$	−**a** + **b** + **c**, **a** − **b** + **c**, **a** + **b** − **c** **a**, **b**, **c** **b** + **c**, **c** + **a**, **a** + **b**
mP	*P*	$-2c \cos\beta < a < c$,§ $\alpha = \gamma = 90^\circ < \beta$	$\beta = 90^\circ \rightarrow oP$ $-2c \cos\beta = a \rightarrow oC$ $a = c \rightarrow oC$	−**b**, **a**, **c** if $a > b$ **a**, **b**, **c** if $a < b < c$ **a**, **c**, −**b** if $b > c$ **a**, −2**c** − **a**, **b** ($a'\sqrt{3} < b'$) **a** + **c**, **a** − **c**, **b** ($a'\sqrt{3} > b'$)
mI	*I*	$-c \cos\beta < a < c$,¶ $\alpha = \gamma = 90^\circ < \beta$	$\beta = 90^\circ \rightarrow oI$ $-c \cos\beta = a \rightarrow oC$ $a = c \rightarrow oF$	−**b**, **a**, **c** if $a > b$ **a**, **b**, **c** if $a < b < c$ **a**, **c**, −**b** if $b > c$ **b**, **c** + **a**, **a** if $b < \lvert\mathbf{c} + \mathbf{a}\rvert$ **c** + **a**, −**b**, **a** if $b > \lvert\mathbf{c} + \mathbf{a}\rvert$ **b**, **a** + **c**, **a** − **c** if $\lvert\mathbf{a} + \mathbf{c}\rvert > b$ **a** + **c**, **b**, **c** − **a** if $\lvert\mathbf{a} + \mathbf{c}\rvert < b < \lvert\mathbf{a} - \mathbf{c}\rvert$ **a** + **c**, **a** − **c**, **b** if $b > \lvert\mathbf{a} - \mathbf{c}\rvert$
		but not††	$a^2 + b^2 = c^2$, $a^2 + ac \cos\beta = b^2 \rightarrow hR$	**a**, (**a** − **b** − **c**)/2, (**a** + **b** − **c**)/2 ($\alpha' < 60^\circ$)
		nor	$a^2 + b^2 = c^2$, $b^2 + ac \cos\beta = a^2 \rightarrow hR$	**a**, (**a** + **b** + **c**)/2, (**a** − **b** + **c**)/2 ($60^\circ < \alpha' < 90^\circ$)
		nor nor	$c^2 + 3b^2 = 9a^2$, $c = -3a \cos\beta \rightarrow hR$ $a^2 + 3b^2 = 9c^2$, $a = -3c \cos\beta \rightarrow hR$	−**a**, (**a** − **b** + **c**)/2, (**a** + **b** + **c**)/2 ($90^\circ < \alpha' < \omega$)‡ −**c**, (**a** + **b** + **c**)/2, (**a** − **b** + **c**)/2 ($\omega < \alpha'$)‡

† The labelling of the basis vectors according to their length is the reason for unconventional Hermann–Mauguin symbols: for example, the Hermann–Mauguin symbol *Pmna* may be changed to *Pncm*, *Pbmn*, *Pman*, *Pcnm* or *Pnmb*. Analogous facts apply to the *oI*, *oC*, *oF*, *mP* and *mI* Bravais types of lattices. ‡ $\omega = \arccos(-1/3) = 109^\circ 28' 16''$. § This means that **a**, **c** are the shortest non-coplanar lattice vectors in their plane. ¶ This means that **a**, **c** are the shortest non-coplanar lattice vectors in their plane on condition that the cell (**a**, **b**, **c**) is body-centred. †† The reason that the limiting cases of *hR* lattices require two additional equalities is that *hR* lattices have only two independent parameters (a, α), whereas *mI* lattices have four (a, b, c, β). A similar situation holds for the transition from anorthic (triclinic) to monoclinic lattices. See Fig. 3.1.4.3.

(i) the centring of (**a**, **b**, **c**) agrees with the centring mode given in column 2 in the *i*th entry, and
(ii) the parameters of the cell (**a**, **b**, **c**) fulfil the conditions listed in column 3 in the *i*th entry of Table 3.1.4.1.

For most entries the conditions contain one or more signs of type $<$ or $\neq$. If one of these signs is replaced by the equality sign, a Bravais type of higher symmetry is obtained. These limiting cases are listed in column 4. A particular situation occurs for the Bravais type *mI*. The conditions given for this type in the first two lines of column 3 exclude the limiting cases *oI*, *oC* and *oF* but not *hR*. The latter case is excluded if none of the four pairs of equalities listed in column 4 is satisfied.

In the present section a cell of an *oP*, *oI* or *oF* lattice is considered conventional if it satisfies not only the conditions given in column 2 of Table 3.1.2.2 but also $a < b < c$. Similarly, the additional requirement $a < b$ is made for *oC* and the additional requirements $a < c$ and $\beta > 90^\circ$ for *mP* and *mI*. Column 5 gives a conventional basis (**a**′, **b**′, **c**′) for the limiting case expressed in terms of the conventional basis (**a**, **b**, **c**) for the original Bravais type. The basis is chosen such that handedness is conserved, *i.e.* all bases considered in this section may be regarded as right-handed. Lattices of the same type obtained from a given original Bravais type by a different limit condition differ in the shape of their conventional cell. For example, both limit conditions for the

original type *oP* lead to lattices of type *tP* with axial ratios $c'/a' > 1$ and < 1, respectively, as shown in column 5.

The following examples illustrate the meaning of the information on limiting cases given in Table 3.1.4.1.

(1) Consider the original Bravais type *oF*. If a face-centred cell satisfies $\alpha = \beta = \gamma = 90°$ and $a < b = c$, the lattice will be of type *tI* with conventional basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = [(\mathbf{b} + \mathbf{c})/2, (\mathbf{c} - \mathbf{b})/2, \mathbf{a}]$ and axial ratio $c'/a' < 1$.

(2) Consider the original Bravais type *mI*. If a body-centred cell satisfies $-c \cos \beta < a < c$, $\alpha = \gamma = 90° < \beta$, $a^2 + b^2 = c^2$ and $a^2 + ac \cos \beta = b^2$, the lattice will be of type *hR* with conventional basis $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = [\mathbf{a}, (\mathbf{a} - \mathbf{b} - \mathbf{c})/2, (\mathbf{a} + \mathbf{b} - \mathbf{c})/2]$ and rhombohedral angle $\alpha' < 60°$.

The limiting cases given in Table 3.1.4.1 are illustrated in Fig. 3.1.4.3.

Figures similar to Fig. 3.1.4.3 were first published by Hosoya (1979) and, independently, by Klemm (1982). The additions made to this section in this present edition are based on Grimmer (2015).

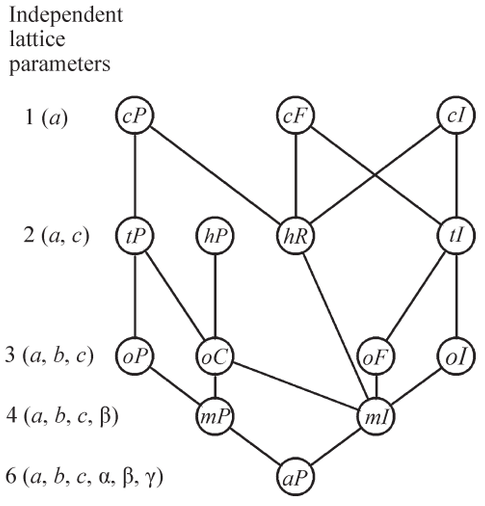


Figure 3.1.4.3
The Bravais-lattice type of the three-dimensional lattice at the upper end of a line is a limiting case of the type at the lower end.

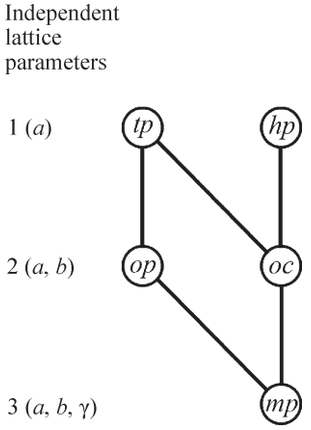


Figure 3.1.4.4
The Bravais-lattice type of the two-dimensional lattice at the upper end of a line is a limiting case of the type at the lower end.

Table 3.1.4.2
Conventional cells for the five two-dimensional Bravais types of lattices and their limiting cases

The centring mode of the cell, *p* or *c*, is indicated in the symbol of the Bravais type.

Bravais type of lattice	Conditions	Limiting cases	Conventional basis $(\mathbf{a}', \mathbf{b}')$ for limiting case
hp	$a = b$, $\gamma = 120°$		
tp	$a = b$, $\gamma = 90°$		
oc	$a < b \neq a\sqrt{3}$, $\gamma = 90°$	$a = b \rightarrow tp$ $a\sqrt{3} = b \rightarrow hp$	$(\mathbf{a} + \mathbf{b})/2, (\mathbf{b} - \mathbf{a})/2$ $\mathbf{a}, (\mathbf{b} - \mathbf{a})/2$
op	$a < b$, $\gamma = 90°$	$a = b \rightarrow tp$	$\mathbf{a}, \mathbf{b}$
mp	$-2b \cos \gamma < a < b$, $90° < \gamma$	$\gamma = 90° \rightarrow op$ $-2b \cos \gamma = a \rightarrow oc$ $a = b \rightarrow oc$	$\mathbf{a}, \mathbf{b}$ $\mathbf{a}, 2\mathbf{b} + \mathbf{a}$ $(a'\sqrt{3} < b')$ $\mathbf{a} + \mathbf{b}, \mathbf{b} - \mathbf{a}$ $(a'\sqrt{3} > b')$

Conventional cells for the five Bravais types of two-dimensional lattices are described and illustrated in Table 3.1.2.1. The conditions given in column 2 of this table are necessary but not always sufficient. Consider the Bravais type whose symbol appears in Table 3.1.4.2 in the *i*th entry of column 1. A two-dimensional lattice **L** is of this Bravais type if and only if there exists a cell $(\mathbf{a}, \mathbf{b})$ with centring mode indicated by the second letter of the Bravais-type symbol and which satisfies the conditions given in the *i*th entry of column 2.

The conditions in the last three entries of column 2 contain one or more signs of type $<$ or $\neq$. If one of these signs is replaced by the equality sign, a Bravais type of higher symmetry is obtained. These limiting cases are listed in column 3 of Table 3.1.4.2. Column 4 gives a conventional basis for the limiting case expressed in terms of the conventional basis for the original Bravais type.

Consider, for example, the original Bravais type *mp*. If a primitive cell satisfies $-2b \cos \gamma = a < b$ and $\gamma > 90°$, the lattice will be of type *oc* with conventional basis $(\mathbf{a}', \mathbf{b}') = (\mathbf{a}, 2\mathbf{b} + \mathbf{a})$ and cell parameters satisfying $a'\sqrt{3} < b'$.

The limiting cases given in Table 3.1.4.2 are illustrated in Fig. 3.1.4.4.

3.1.4.5. Conventional characters

Lattice characters were defined in Section 3.1.4.2 by dividing the Niggli image of a certain Bravais type $\mathscr{T}$ into components. Doing the same – instead of with the Niggli points – with the parameters of conventional cells[7] of lattices of the Bravais type $\mathscr{T}$ we obtain a division of the range[8] of these parameters into components. This leads to a further division of lattices of the Bravais type $\mathscr{T}$ into equivalence classes. We call these classes – in analogy to the Niggli characters – *conventional characters*. There are 22 of them.

Two lattices of the same Bravais type belong to the same conventional character if and only if one lattice can be deformed into the other in such a way that the conventional parameters of the deformed lattice change *continuously* from the initial to the final position without change of the Bravais type. The word 'continuously' cannot be replaced by the stronger term 'linearly' because the range of conventional parameters of the monoclinic centred lattices is not convex.

[7] For *aP* lattices, these parameters are derived from the Niggli point [see (3.1.4.2)].
[8] This range is a subset of $\mathbb{E}_k$, where $k \leq 6$.

Table 3.1.4.3
Conventional characters

Bravais type of lattice	Conditions	Conventional character
cP		{3}
cI		{5}
cF		{1}
tP	$a < c$	{11}
	$c < a$	{21}
tI	$a < c/\sqrt{2}$	{15}
	$c/\sqrt{2} < a < c$	{7}
	$c < a$	{6, 18}
oP		{32}
oI		{8, 19, 42}
oF		{16, 26}
oC	$b < a\sqrt{3}$	{13, 23}
	$a\sqrt{3} < b$	{36, 38, 40}
hP		{12, 22}
hR†	$\alpha < 60^\circ$	{9}
	$60^\circ < \alpha < 90^\circ$	{2}
	$90^\circ < \alpha < \omega$‡	{4}
	$\omega < \alpha$	{24}
mP		{33, 34, 35}
mC		{10, 14, 17, 20, 25, 27, 28, 29, 30, 37, 39, 41, 43}
aP	$\alpha < 90^\circ$	{31}
	$90^\circ \leq \alpha$	{44}

† The angle α refers to the rhombohedral description of the *hR* lattices. ‡ $\omega = \arccos(-1/3) = 109^\circ 28' 16''$.

Conventional characters form a superdivision of the lattice characters. Therefore, no special notation of conventional characters need be invented: we write them simply as sets of lattice characters which constitute the conventional character. Denoting the lattice characters by integral numbers from 1 to 44 (according to the convention in Section 3.1.3.5), we obtain for the conventional characters symbols like {8, 19, 42} or {7}.

Conventional characters are described in Table 3.1.4.3.

3.1.4.6. Sublattices

A sublattice $\mathbf{L}'$ of an n-dimensional lattice $\mathbf{L}$ is a proper subset of $\mathbf{L}$ which itself is a lattice of the same dimension as $\mathbf{L}$. A sublattice $\mathbf{L}'$ of $\mathbf{L}$ causes a decomposition of the set $\mathbf{L}$ into, say, i mutually congruent sublattices, $\mathbf{L}'$ itself being one of them (Fig. 3.1.4.5). The number i is called the *index* of the sublattice $\mathbf{L}'$ and indicates how many times $\mathbf{L}'$ is 'diluted' with respect to $\mathbf{L}$.

Sublattices are defined in a natural way in those lattices that have centred conventional cells, being generated by the vertices of these cells ('decentring'). They are primitive and belong to the same crystal family as the given lattice. Thus, in the *cI*, *cF*, *tI*, *oI*, *oF*, *oC*, *mC* and *hR*[9] lattices, we can meet sublattices of indices 2, 4, 2, 2, 4, 2, 2 and 3, respectively.

Theoretically (though hardly in crystallographic practice), the Bravais type of centred lattices can also be determined by testing all their sublattices with the suspected index and finding in any of these sublattices the Niggli cell.

All sublattices of index i of an n-dimensional lattice $\mathbf{L}$ can be constructed by a procedure suggested by Cassels (1971). If $\mathbf{a}_1, \ldots, \mathbf{a}_n$ is a primitive basis of the lattice $\mathbf{L}$ then primitive bases $\mathbf{a}'_1, \ldots, \mathbf{a}'_n$ of all sublattices of index i of the lattice $\mathbf{L}$ can be found by the relations

$$[\mathbf{a}'_1, \ldots, \mathbf{a}'_n] = [\mathbf{a}_1, \ldots, \mathbf{a}_n]\boldsymbol{R}^T,$$

[9] When choosing their hexagonal description.

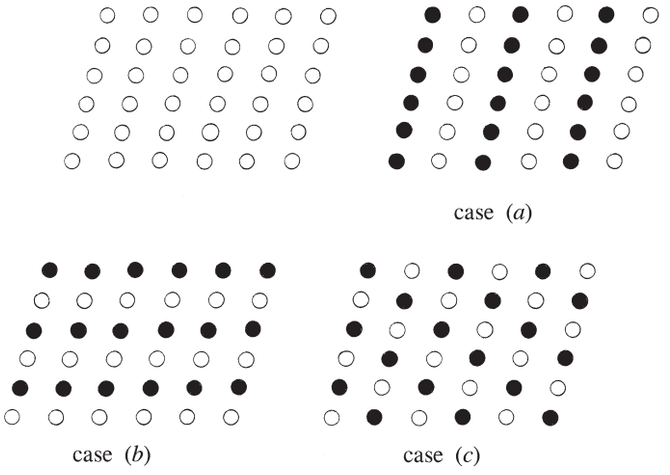


Figure 3.1.4.5
Three possible decompositions of a two-dimensional lattice $\mathbf{L}$ into sublattices of index 2.

where the matrix $\boldsymbol{R} = [r_{ij}]$ fulfils

$$\begin{aligned} 0 &= r_{ij} && \text{for} \quad 1 \leq i < j \leq n, \\ 0 &\leq r_{ij} < r_{jj} && \text{for} \quad 1 \leq j < i \leq n, \\ r_{11} \ldots r_{nn} &= i. \end{aligned} \tag{3.1.4.4}$$

The number $D_{n,i}$ of these matrices is equal to the number of decompositions of an n-dimensional lattice $\mathbf{L}$ into sublattices of index i. To determine this number, it is not necessary to construct explicitly the matrices fulfilling (3.1.4.4). The following formulae (Gruber, 1997*b*) can be used:

(i) If $i = p^q$, where $p > 1$ is a prime number, then

$$D_{n,i} = \underbrace{\frac{p^n - 1}{p - 1} \times \frac{p^{n+1} - 1}{p^2 - 1} \times \frac{p^{n+2} - 1}{p^3 - 1} \times \ldots .}_{q \text{ times}}$$

(ii) If $i = p_1^{q_1} \ldots p_m^{q_m}$ ($p_1, \ldots, p_m$ mutually different prime numbers, $m > 1$), we deal with any factor $p_j^{q_j}$ ($j = 1, \ldots, m$) according to point (i) and multiply all these numbers to obtain the number $D_{n,i}$.

For example, for $n = 3$ and $i = 2, 3, 4$ and 6, we obtain for $D_{n,i}$ the values 7, 13, 35 and 91, respectively.

In all considerations so far, the symmetry of the lattice $\mathbf{L}$ was irrelevant. We took $\mathbf{L}$ simply as a set of points and its sublattices as its subsets. [Thus, for illustrating sublattices, the 'triclinic' lattices are most apt; *cf.* 'derivative lattices' in Chapter 13.2 in the 5th (2002) edition of this volume.]

However, this is not exactly the crystallographic point of view. If, for example, the mesh of the lattice $\mathbf{L}$ in Fig. 3.1.4.5 were a square, the sublattices in cases (*a*) and (*b*) would have the same symmetry (though being different subsets of $\mathbf{L}$) and therefore would be considered by crystallographers as one case only. The number $D_{n,i}$ would be reduced. From this aspect, the problem is treated in Chapter 13.1 in the 5th (2002) edition of this volume in group-theoretical terms which are more suitable for this purpose than the set-theory language used here. See also Section 2.1.4 of *International Tables for Crystallography* Volume A1 (2010).

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3.2. Point groups and crystal classes

Th. Hahn, H. Klapper, U. Müller and M. I. Aroyo

3.2.1. Crystallographic and noncrystallographic point groups

By Th. Hahn and H. Klapper

3.2.1.1. Introduction and definitions

A *point group*[1] is a group of symmetry operations all of which leave at least one point unmoved. Thus, all operations containing translations are excluded. Point groups can be subdivided into crystallographic and noncrystallographic point groups. A *crystallographic* point group is a point group that maps a point lattice onto itself. Consequently, rotations and rotoinversions are restricted to the well known crystallographic cases 1, 2, 3, 4, 6 and $\overline{1}$, $\overline{2} = m$, $\overline{3}$, $\overline{4}$, $\overline{6}$ (*cf.* Section 1.2.1); matrices for these symmetry operations are listed in Tables 1.2.2.1 and 1.2.2.2. No such restrictions apply to the *noncrystallographic* point groups.

The numbers of the crystallographic point groups are finite: 2 for one dimension, 10 for two dimensions and 32 for three dimensions. The numbers of noncrystallographic point groups for dimensions $n \geq 2$ are infinite. The two- and three-dimensional crystallographic point groups and their crystal systems are summarized in Tables 3.2.1.1 and 3.2.1.2. They are described in detail in Section 3.2.1.2. The two one-dimensional point groups are discussed in Section 2.1.3.16. The noncrystallographic point groups are treated in Section 3.2.1.4.

Crystallographic point groups occur:

(i) in vector space as symmetries of the external shapes of crystals, *i.e.* of the set of vectors normal to the crystal faces (morphological symmetry); this also includes the symmetries of sets of symmetry-equivalent net planes in crystals (reciprocal-lattice points), fundamental for the theory of X-ray diffraction.

(ii) in point space as site symmetries of points in lattices or in crystal structures and as symmetries of molecules, atomic groups and coordination polyhedra.

General point groups, *i.e.* crystallographic *and* noncrystallographic point groups, occur as:

(iii) symmetries of (rigid) molecules (molecular symmetry):

(iv) symmetries of physical properties of crystals (*e.g.* tensor symmetries); here noncrystallographic point groups with axes of order infinity are of particular importance, as in the symmetries of circles, spheres or rotation ellipsoids:

(v) approximate symmetries of the local environment of a point in a crystal structure, *i.e.* as *local* site symmetries. Examples are sphere-like atoms or ions in crystals, as well as icosahedral atomic groups. These noncrystallographic symmetries, however, are only approximate, even for the close neighbourhood of a site.

A (geometric) *crystal class* (point-group type) is the set of all crystals having the same point-group symmetry. The word 'class', therefore, denotes a classificatory pigeonhole and should not be used as synonymous with the point group of a particular crystal. The symbol of a crystal class is that of the common point group. (For geometric and arithmetic crystal classes of space groups, see Sections 1.3.4.2 and 1.3.4.4.)

Of particular importance for the structure determination of crystals are the 11 *centrosymmetric crystallographic point groups*, because they describe the possible symmetries of the diffraction record of a crystal: $\overline{1}$; $2/m$; mmm; $4/m$; $4/mmm$; $\overline{3}$; $\overline{3}m$; $6/m$; $6/mmm$; $m\overline{3}$; $m\overline{3}m$. This is due to Friedel's rule, which states that, provided anomalous dispersion is neglected, the diffraction record of any crystal is centrosymmetric, even if the crystal is noncentrosymmetric. The symmetry of the diffraction record determines the *Laue class* of the crystal; this is further explained in Chapter 1.6. For a given crystal, its Laue class is obtained if a symmetry centre is added to its point group, as shown in Table 3.2.2.1.

In two dimensions, six 'centrosymmetric' crystallographic point groups and hence six two-dimensional Laue classes exist: 2; 2*mm*; 4; 4*mm*; 6; 6*mm*. These point groups are, for instance, the only possible symmetries of zero-layer X-ray photographs.

Among the centrosymmetric crystallographic point groups in three dimensions, the seven *lattice point groups* (holohedral point groups, *holohedries*) are of special importance because they constitute the possible point symmetries of lattices, *i.e.* the site symmetries of their nodes. In three dimensions, the seven holohedries are: $\overline{1}$; $2/m$; mmm; $4/mmm$; $\overline{3}m$; $6/mmm$; $m\overline{3}m$. Note that $\overline{3}m$ is the point symmetry of the rhombohedral lattice and $6/mmm$ the point symmetry of the hexagonal lattice; both occur in the hexagonal crystal family (*cf.* Chapter 2.1). Point groups that are, within a crystal family, subgroups of a holohedry are called merohedries; they are called specifically hemihedries for subgroups of index 2, tetartohedries for index 4 and ogdohedries for index 8.

In two dimensions, four holohedries exist: 2; 2*mm*; 4*mm*; 6*mm*. Note that the hexagonal crystal family in two dimensions contains only one lattice type, with point symmetry 6*mm*.

Another classification of the crystallographic point groups is that into isomorphism classes. Here all those point groups that have the same kind of group table appear in one class. These isomorphism classes are also known under the name of *abstract point groups*.

There are 18 abstract crystallographic point groups in three dimensions: the point groups in each of the following lines are isomorphous and belong to the same abstract group:

Table 3.2.1.1
The ten two-dimensional crystallographic point groups, arranged according to crystal system

The dashed line separates point groups with different Laue classes within one crystal system.

General symbol	Crystal system				
	Oblique (top) Rectangular (bottom)		Square	Hexagonal	
n	1	2	4	3	6
nmm	m	2*mm*	4*mm*	3*m*	6*mm*

[1] For reasons of simplicity, in this chapter the same term 'point group' is used for a 'particular point group' *and* a 'type of point group'. For space groups, this distinction is explained in Section 1.3.4.1. For a different use of the term 'point group' see Section 1.3.3.1.

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Table 3.2.1.2
The 32 three-dimensional crystallographic point groups, arranged according to crystal system (*cf.* Chapter 2.1)

Full Hermann–Mauguin (left) and Schoenflies symbols (right). The dashed line separates point groups with different Laue classes within one crystal system. A brief introduction to point-group symbols is provided in Hahn & Klapper (2005).

General symbol	Crystal system									
	Triclinic		Monoclinic (top) Orthorhombic (bottom)		Tetragonal		Trigonal		Hexagonal		Cubic	
n	1	C_1	2	C_2	4	C_4	3	C_3	6	C_6	23	T
$\overline{n}$	$\overline{1}$	C_i	$m \equiv \overline{2}$	C_s	$\overline{4}$	S_4	$\overline{3}$	C_{3i}	$\overline{6} \equiv 3/m$	C_{3h}	–	–
n/m			$2/m$	C_{2h}	$4/m$	C_{4h}	–	–	$6/m$	C_{6h}	$2/m\overline{3}$	T_h
$n22$			222	D_2	422	D_4	32	D_3	622	D_6	432	O
nmm			$mm2$	C_{2v}	$4mm$	C_{4v}	$3m$	C_{3v}	$6mm$	C_{6v}	–	–
$\overline{n}2m$			–	–	$\overline{4}2m$	D_{2d}	$\overline{3}2/m$	D_{3d}	$\overline{6}2m$	D_{3h}	$\overline{4}3m$	T_d
$n/m\,2/m\,2/m$			$2/m\,2/m\,2/m$	D_{2h}	$4/m\,2/m\,2/m$	D_{4h}	–	–	$6/m\,2/m\,2/m$	D_{6h}	$4/m\,\overline{3}\,2/m$	O_h

Order 1: 1
2: $\overline{1}$, 2, m
3: 3
4: $2/m$, 222, $mm2$
4: 4, $\overline{4}$
6: $\overline{3}$, 6, $\overline{6}$
6: 32, $3m$
8: mmm
8: $4/m$
Order 8: 422, $4mm$, $\overline{4}2m$
12: $6/m$
12: $\overline{3}m$, 622, $6mm$, $\overline{6}2m$
12: 23
16: $4/mmm$
24: $6/mmm$
24: $m\overline{3}$
24: 432, $\overline{4}3m$
48: $m\overline{3}m$.

In two dimensions, the ten crystallographic point groups form nine abstract groups; the groups 2 and m are isomorphous and belong to the same abstract group, the remaining eight point groups correspond to one abstract group each.

3.2.1.2. Crystallographic point groups

3.2.1.2.1. Description of point groups

In crystallography, point groups usually are described

(i) by means of their Hermann–Mauguin or Schoenflies symbols;
(ii) by means of their stereographic projections;
(iii) by means of the matrix representations of their symmetry operations, frequently listed in the form of Miller indices (hkl) of the equivalent general crystal faces;
(iv) by means of drawings of actual crystals, natural or synthetic.

Descriptions (i) through (iii) are given in this section, whereas for crystal drawings and actual photographs reference is made to textbooks of crystallography and mineralogy [Buerger (1956, ch. 10) and Phillips (1971, chs. 3, 4 and 6) are particularly rich in pictures of crystal morphologies]; this also applies to the construction and the properties of the stereographic projection.

In Tables 3.2.3.1 and 3.2.3.2, the two- and three-dimensional crystallographic point groups are listed and described. The tables are arranged according to crystal systems and Laue classes. Within each crystal system and Laue class, the sequence of the point groups corresponds to that in the space-group tables of this volume: pure rotation groups are followed by groups containing reflections, rotoinversions and inversions. The holohedral point group is always given last.

In Tables 3.2.3.1 and 3.2.3.2, some point groups are described in *two or three versions*, in order to bring out the relations to the corresponding space groups (*cf.* Section 2.1.3.2):

(*a*) The three monoclinic point groups 2, m and $2/m$ are given with two settings, one with 'unique axis b' and one with 'unique axis c'.
(*b*) The two point groups $\overline{4}2m$ and $\overline{6}m2$ are described for two orientations with respect to the crystal axes, as $\overline{4}2m$ and $\overline{4}m2$ and as $\overline{6}m2$ and $\overline{6}2m$.
(*c*) The five trigonal point groups 3, $\overline{3}$, 32, $3m$ and $\overline{3}m$ are treated with two axial systems, 'hexagonal axes' and 'rhombohedral axes'.
(*d*) The hexagonal-axes description of the three trigonal point groups 32, $3m$ and $\overline{3}m$ is given for two orientations, as 321 and 312, as $3m1$ and $31m$, and as $\overline{3}m1$ and $\overline{3}1m$; this applies also to the two-dimensional point group $3m$.

The presentation of the point groups is similar to that of the space groups in Part 2. The *headline* contains the short Hermann–Mauguin and the Schoenflies symbols. The full Hermann–Mauguin symbol, if different, is given below the short symbol. No Schoenflies symbols exist for two-dimensional groups. For an explanation of the symbols see Sections 1.4.1 and 2.1.3.4, and Chapter 3.3.

Next to the headline, a pair of *stereographic projections* is given. The diagram on the left displays a general crystal or point form, that on the right shows the 'framework of symmetry elements'. Except as noted below, the c axis is always normal to the plane of the figure, the a axis points down the page and the b axis runs horizontally from left to right. For the five trigonal point groups, the c axis is normal to the page only for the description with 'hexagonal axes'; if described with 'rhombohedral axes', the direction [111] is normal and the positive a axis slopes towards the observer. The conventional coordinate systems used for the various crystal systems are listed in Table 2.1.1.1 and illustrated in Figs. 2.1.3.1 to 2.1.3.10.

In the *right-hand projection*, the graphical symbols of the symmetry elements are the same as those used in the space-group diagrams; they are listed in Chapter 2.1. Note that the symbol of a symmetry centre, a small circle, is also used for a face pole in the left-hand diagram. Mirror planes are indicated by heavy solid lines or circles; thin lines are used for the projection circle, for symmetry axes in the plane and for some special zones in the cubic system.

In the *left-hand projection*, the projection circle and the coordinate axes are indicated by thin solid lines, as are again some special zones in the cubic system. The dots and circles in this projection can be interpreted in two ways.

(i) As *general face poles*, where they represent general crystal faces which form a polyhedron, the 'general crystal form' (face form) {hkl} of the point group (see below). In two dimensions, edges, edge poles, edge forms and polygons take the place of faces, face poles, crystal forms (face forms) and polyhedra in three dimensions.

Face poles marked as dots lie above the projection plane and represent faces which intersect the positive c axis[2] (positive Miller index l), those marked as circles lie below the projection plane (negative Miller index l). In two dimensions, edge poles always lie on the pole circle.

(ii) As *general points* (centres of atoms) that span a polyhedron or polygon, the 'general crystallographic point form' x, y, z. This interpretation is of interest in the study of coordination polyhedra, atomic groups and molecular shapes. The polyhedron or polygon of a point form is dual to the polyhedron of the corresponding crystal form.[3]

The general, special and limiting *crystal forms* and *point forms* constitute the main part of the table for each point group. The theoretical background is given below in Section 3.2.1.2.2, *Crystal and point forms* and an explanation of the listed data is to be found in Section 3.2.1.2.3, *Description of crystal and point forms.*

The last entry for each point group contains the *Symmetry of special projections*, *i.e.* the plane point group that is obtained if the three-dimensional point group is projected along a symmetry direction. The special projection directions are the same as for the space groups; they are listed in Section 2.1.3.14. The relations between the axes of the three-dimensional point group and those of its two-dimensional projections can easily be derived with the help of the stereographic projection. No projection symmetries are listed for the two-dimensional point groups.

Note that the symmetry of a projection along a certain direction may be higher than the symmetry of the crystal face normal to that direction. For example, in point group $\overline{1}$ all faces have face symmetry 1, whereas projections along any direction have symmetry 2; in point group 422, the faces (001) and (00$\overline{1}$) have face symmetry 4, whereas the projection along [001] has symmetry 4*mm*.

3.2.1.2.2. Crystal and point forms

For a point group $\mathcal{P}$ a *crystal form* is a set of all symmetry-equivalent faces; a *point form* is a set of all symmetry-equivalent points. Crystal and point forms in point groups correspond to 'crystallographic orbits' in space groups; *cf.* Sections 1.1.7 and 1.4.4.1.

Two kinds of crystal and point forms with respect to $\mathcal{P}$ can be distinguished. They are defined as follows:

(i) *General form*: A *face* is called 'general' if only the identity operation transforms the face onto itself. Each complete set of symmetry-equivalent 'general faces' is a *general crystal form.* The *multiplicity* of a general form, *i.e.* the number of its faces, is the order of $\mathcal{P}$. In the stereographic projection, the poles of general faces do *not* lie on symmetry elements of $\mathcal{P}$.

A *point* is called 'general' if its *site symmetry*, *i.e.* the group of symmetry operations that transforms this point onto itself, is 1. A *general point form* is a complete set of symmetry-equivalent 'general points'.

(ii) *Special form*: A *face* is called 'special' if it is transformed onto itself by at least one symmetry operation of $\mathcal{P}$, in addition to the identity. Each complete set of symmetry-equivalent 'special faces' is called a *special crystal form.* The *face symmetry* of a special face is the group of symmetry operations that transforms this face onto itself; it is a subgroup of $\mathcal{P}$. The multiplicity of a special crystal form is the multiplicity of the general form divided by the order of the face-symmetry group. In the stereographic projection, the poles of special faces lie on symmetry elements of $\mathcal{P}$. The Miller indices of a special crystal form obey restrictions like {hk0}, {hhl}, {100}.

A *point* is called 'special' if its *site symmetry* is higher than 1. A special point form is a complete set of symmetry-equivalent 'special points'. The multiplicity of a special point form is the multiplicity of the general form divided by the order of the site-symmetry group. It is thus the same as that of the corresponding special crystal form. The coordinates of the points of a special point form obey restrictions, like x, y, 0; x, x, z; x, 0, 0.

In two dimensions, point groups 1, 2, 3, 4 and 6 and, in three dimensions, point groups 1 and $\overline{1}$ have no special crystal forms.

General and special crystal and point forms can be represented by their sets of equivalent Miller indices {hkl} and point coordinates x, y, z. Each set of these 'triplets' stands for infinitely many crystal forms or point forms which are obtained by independent variation of the values and signs of the Miller indices h, k, l or the point coordinates x, y, z.

It should be noted that for crystal forms, owing to the well known 'law of rational indices', the indices h, k, l must be integers; no such restrictions apply to the coordinates x, y, z, which can be rational or irrational numbers.

Example

In point group 4, the general crystal form {hkl} stands for the set of all possible tetragonal pyramids, pointing either upwards or downwards, depending on the sign of l; similarly, the general point form x, y, z includes all possible squares, lying either above or below the origin, depending on the sign of z. For the limiting cases $l = 0$ or $z = 0$, see below.

In order to survey the infinite number of possible forms of a point group, they are classified into *Wyckoff positions of crystal and point forms,* for short *Wyckoff positions*. This name has been chosen in analogy to the Wyckoff positions of space groups; *cf.* Sections 1.4.4.2 and 2.1.3.11. In point groups, the term 'position' can be visualized as the position of the face poles and points in the stereographic projection. Each 'Wyckoff position' is labelled by a *Wyckoff letter*.

Definition

A 'Wyckoff position of crystal and point forms' consists of all those crystal forms (point forms) of a point group $\mathcal{P}$ for which the face poles (points) are positioned on the same set of conjugate symmetry elements of $\mathcal{P}$; *i.e.* for each face (point) of one form there is one face (point) of every other form of the same 'Wyckoff position' that has exactly the same face (site) symmetry.

Each point group contains one 'general Wyckoff position' comprising all *general* crystal and point forms. In addition, up to two 'special Wyckoff positions' may occur in two dimensions and up to six in three dimensions. They are characterized by the different sets of conjugate face and site symmetries and correspond to the seven positions of a pole in the interior, on the three edges, and at the three vertices of the so-called 'characteristic triangle' of the stereographic projection.

Examples

(1) All tetragonal pyramids {hkl} and tetragonal prisms {hk0} in point group 4 have face symmetry 1 and belong to the same general 'Wyckoff position' 4*b*, with Wyckoff letter *b*.

[2] This does not apply to 'rhombohedral axes': here the positive directions of all three axes slope upwards from the plane of the paper: *cf.* Fig. 2.1.3.9.

[3] Dual polyhedra have the same number of edges, but the numbers of faces and vertices are interchanged; *cf.* textbooks of geometry.

(2) All tetragonal pyramids *and* tetragonal prisms in point group 4*mm* belong to two special 'Wyckoff positions', depending on the orientation of their face-symmetry groups *m* with respect to the crystal axes: For the 'oriented face symmetry' *.m.*, the forms {*h*0*l*} and {100} belong to Wyckoff position 4*c*; for the oriented face symmetry *..m*, the forms {*hhl*} and {110} belong to Wyckoff position 4*b*. The face symmetries *.m.* and *..m* are not conjugate in point group 4*mm*. For the analogous 'oriented site symmetries' in space groups, see Section 2.1.3.12.

It is instructive to subdivide the crystal forms (point forms) of one Wyckoff position further, into *characteristic* and *noncharacteristic* forms. For this, one has to consider two symmetries that are connected with each crystal (point) form:

(i) the point group $\mathcal{P}$ by which a form is generated (*generating point group*), *i.e.* the point group in which it occurs;

(ii) the full symmetry (inherent symmetry) of a form (considered as a polyhedron by itself), here called eigensymmetry $\mathscr{E}$. The *eigensymmetry point group* $\mathscr{E}$ is either the generating point group itself or a supergroup of it.

Examples

(1) Each tetragonal pyramid {*hkl*} ($l \neq 0$) of Wyckoff position 4*b* in point group 4 has generating symmetry 4 and eigensymmetry 4*mm*; each tetragonal prism {*hk*0} of the same Wyckoff position has generating symmetry 4 again, but eigensymmetry 4/*mmm*.

(2) A cube {100} may have generating symmetry 23, $m\bar{3}$, 432, $\bar{4}3m$ or $m\bar{3}m$, but its eigensymmetry is always $m\bar{3}m$.

The eigensymmetries and the generating symmetries of the 47 crystal forms (point forms) are listed in Table 3.2.1.3. With the help of this table, one can find the various point groups in which a given crystal form (point form) occurs, as well as the face (site) symmetries that it exhibits in these point groups; for experimental methods see Sections 3.2.2.2 and 3.2.2.3. Diagrams of the 47 crystal forms are presented in Fig. 3.2.1.1.

With the help of the two groups $\mathcal{P}$ and $\mathscr{E}$, each crystal or point form occurring in a particular point group can be assigned to one of the following two categories:

(i) *characteristic* form, if eigensymmetry $\mathscr{E}$ and generating symmetry $\mathcal{P}$ are the same;

(ii) *noncharacteristic* form, if $\mathscr{E}$ is a proper supergroup of $\mathcal{P}$.

The importance of this classification will be apparent from the following examples.

Examples

(1) A pedion and a pinacoid are noncharacteristic forms in all crystallographic point groups in which they occur:

(2) all other crystal or point forms occur as characteristic forms in their eigensymmetry group $\mathscr{E}$;

(3) a tetragonal pyramid is noncharacteristic in point group 4 and characteristic in 4*mm*;

(4) a hexagonal prism can occur in nine point groups (12 Wyckoff positions) as a noncharacteristic form; in 6/*mmm*, it occurs in two Wyckoff positions as a characteristic form.

The general forms of the 13 point groups with no, or only one, symmetry direction ('monoaxial groups') $1, 2, 3, 4, 6, \bar{1}, m, \bar{3}, \bar{4}, \bar{6} = 3/m, 2/m, 4/m, 6/m$ are always noncharacteristic, *i.e.* their eigensymmetries are enhanced in comparison with the generating point groups. The general positions of the other 19 point groups always contain characteristic crystal forms that may be used to determine the point group of a crystal uniquely (*cf.* Section 3.2.2).[4]

So far, we have considered the occurrence of one crystal or point form in different point groups and different Wyckoff positions. We now turn to the occurrence of different kinds of crystal or point forms in one and the same Wyckoff position of a particular point group.

In a Wyckoff position, crystal forms (point forms) of different eigensymmetries may occur; the crystal forms (point forms) with the lowest eigensymmetry (which is always well defined) are called *basic forms* (German: *Grundformen*) of that Wyckoff position. The crystal and point forms of higher eigensymmetry are called *limiting forms* (German: *Grenzformen*) (*cf.* Table 3.2.1.3). These forms are always noncharacteristic.

Limiting forms[5] occur for certain restricted values of the Miller indices or point coordinates. They always have the same multiplicity and oriented face (site) symmetry as the corresponding basic forms because they belong to the same Wyckoff position. The enhanced eigensymmetry of a limiting form may or may not be accompanied by a change in the topology[6] of its polyhedra, compared with that of a basic form. In every case, however, the name of a limiting form is different from that of a basic form.

The face poles (or points) of a limiting form lie on symmetry elements of a supergroup of the point group that are not symmetry elements of the point group itself. There may be several such supergroups.

Examples

(1) In point group 4, the (noncharacteristic) crystal forms {*hkl*} ($l \neq 0$) (tetragonal pyramids) of eigensymmetry 4*mm* are basic forms of the general Wyckoff position 4*b*, whereas the forms {*hk*0} (tetragonal prisms) of higher eigensymmetry 4/*mmm* are 'limiting general forms'. The face poles of forms {*hk*0} lie on the horizontal mirror plane of the supergroup 4/*m*.

(2) In point group 4*mm*, the (characteristic) special crystal forms {*h*0*l*} with eigensymmetry 4*mm* are 'basic forms' of the special Wyckoff position 4*c*, whereas {100} with eigensymmetry 4/*mmm* is a 'limiting special form'. The face poles of {100} are located on the intersections of the vertical mirror planes of the point group 4*mm* with the horizontal mirror plane of the supergroup 4/*mmm*, *i.e.* on twofold axes of 4/*mmm*.

Whereas basic and limiting forms belonging to one 'Wyckoff position' are always clearly distinguished, closer inspection shows that a Wyckoff position may contain different 'types' of limiting forms. We need, therefore, a further criterion to classify the limiting forms of one Wyckoff position into types: A *type of limiting form of a Wyckoff position* consists of all those limiting forms for which the face poles (points) are located on the same set of additional conjugate symmetry elements of the holohedral point group (for the trigonal point groups, the hexagonal holo-

[4] For a survey of these relations, as well as of the 'limiting forms', it is helpful to consider the (seven) *normalizers* of the crystallographic point groups in the group of all rotations and reflections (orthogonal group, sphere group); normalizers of the crystallographic and noncrystallographic point groups are listed in Tables 3.5.4.1 and 3.5.4.2.

[5] The treatment of 'limiting forms' in the literature is quite ambiguous. In some textbooks, limiting forms are omitted or treated as special forms in their own right: other authors define only limiting *general* forms and consider limiting *special* forms as if they were new special forms. For additional reading, see P. Niggli (1941, pp. 80–98).

[6] The topology of a polyhedron is determined by the numbers of its vertices, edges and faces, by the number of vertices of each face and by the number of faces meeting in each vertex.

Table 3.2.1.3
The 47 crystallographic face and point forms, their names, eigensymmetries, and their occurrence in the crystallographic point groups (generating point groups)

The oriented face (site) symmetries of the forms are given in parentheses after the Hermann–Mauguin symbol (column 6); a symbol such as *mm*2(*.m.*, *m..*) indicates that the form occurs in point group *mm*2 twice, with face (site) symmetries *.m.* and *m...* Basic (general and special) forms are printed in bold face, limiting (general and special) forms in normal type. The various settings of point groups 32, 3*m*, $\bar{3}m$, $\bar{4}2m$ and $\bar{6}m2$ are connected by braces. The 47 crystal forms are shown in Fig. 3.2.1.1. (Note that the numbering of the forms in column 1 does not correspond to the numbering used in Fig. 3.2.1.1.)

No.	Crystal form	Point form	Number of faces or points	Eigensymmetry	Generating point groups with oriented face (site) symmetries between parentheses
1	Pedion or monohedron	Single point	1	∞m	**1(1)**; **2(2)**; ***m*(*m*)**; **3(3)**; **4(4)**; **6(6)**; ***mm*2(*mm*2)**; **4*mm*(4*mm*)**; **3*m*(3*m*)**; **6*mm*(6*mm*)**
2	Pinacoid or parallelohedron	Line segment through origin	2	$\frac{\infty}{m}m$	$\bar{1}$**(1)**; 2(1); *m*(1); $\frac{\mathbf{2}}{\boldsymbol{m}}$**(2, *m*)**; **222(2.., .2., ..2)**; *mm*2(*.m.*, *m..*); ***mmm*(2*mm*, *m*2*m*, *mm*2)**; $\bar{4}$**(2..)**; $\frac{\mathbf{4}}{\boldsymbol{m}}$**(4..)**; **422(4..)**; $\left\{\begin{matrix}\bar{4}2m(2.mm)\\ \bar{4}m2(2mm.)\end{matrix}\right.$; $\frac{\mathbf{4}}{\boldsymbol{m}}$***mm*(4*mm*)**; $\bar{3}$**(3)**; $\left\{\begin{matrix}321(3..)\\ 312(3..)\\ 32\ \ (3.)\end{matrix}\right.$ $\left\{\begin{matrix}\bar{3}m1(3m.)\\ \bar{3}1m(3.m)\\ \bar{3}m\ \ (3m)\end{matrix}\right.$; $\bar{6}$**(3..)**; $\frac{\mathbf{6}}{\boldsymbol{m}}$**(6..)**; **622(6..)**; $\left\{\begin{matrix}\bar{6}m2(3m.)\\ \bar{6}2m(3.m)\end{matrix}\right.$; $\frac{\mathbf{6}}{\boldsymbol{m}}$***mm*(6*mm*)**
3	Sphenoid, dome, or dihedron	Line segment	2	*mm*2	**2(1)**; ***m*(1)**; ***mm*2(*.m.*, *m..*)**
4	Rhombic disphenoid or rhombic tetrahedron	Rhombic tetrahedron	4	222	**222(1)**
5	Rhombic pyramid	Rectangle	4	*mm*2	***mm*2(1)**
6	Rhombic prism	Rectangle through origin	4	*mmm*	**2/*m*(1)**; 222(1)†; *mm*2(1); ***mmm*(*m..*, *.m.*, *..m*)**
7	Rhombic dipyramid	Rectangular prism	8	*mmm*	***mmm*(1)**
8	Tetragonal pyramid	Square	4	4*mm*	**4(1)**; **4*mm*(*..m*, *.m.*)**
9	Tetragonal disphenoid or tetragonal tetrahedron	Tetragonal tetrahedron	4	$\bar{4}2m$	$\bar{4}$**(1)**; $\left\{\begin{matrix}\bar{4}2m(..m)\\ \bar{4}m2(.m.)\end{matrix}\right.$
10	Tetragonal prism	Square through origin	4	$\frac{4}{m}mm$	4(1); $\bar{4}$(1); $\frac{\mathbf{4}}{\boldsymbol{m}}$**(*m..*)**; **422(..2, .2.)**; 4*mm*(*..m*, *.m.*); ‡$\left\{\begin{matrix}\bar{4}2m(.2.)\ \text{and}\ \bar{4}2m(..m)\\ \bar{4}m2(..2)\ \text{and}\ \bar{4}m2(.m.)\end{matrix}\right.$; $\frac{\mathbf{4}}{\boldsymbol{m}}$***mm*(*m.m*2, *m*2*m.*)**
11	Tetragonal trapezohedron	Twisted tetragonal antiprism	8	422	**422(1)**
12	Ditetragonal pyramid	Truncated square	8	4*mm*	**4*mm*(1)**
13	Tetragonal scalenohedron	Tetragonal tetrahedron cut off by pinacoid	8	$\bar{4}2m$	$\left\{\begin{matrix}\bar{4}2m(1)\\ \bar{4}m2(1)\end{matrix}\right.$
14	Tetragonal dipyramid	Tetragonal prism	8	$\frac{4}{m}mm$	$\frac{\mathbf{4}}{\boldsymbol{m}}$**(1)**; 422(1)†; $\left\{\begin{matrix}\bar{4}2m(1)\\ \bar{4}m2(1)\end{matrix}\right.$; $\frac{\mathbf{4}}{\boldsymbol{m}}$***mm*(*.m*, *.m.*)**
15	Ditetragonal prism	Truncated square through origin	8	$\frac{4}{m}mm$	422(1); 4*mm*(1); $\left\{\begin{matrix}\bar{4}2m(1)\\ \bar{4}m2(1)\end{matrix}\right.$; $\frac{\mathbf{4}}{\boldsymbol{m}}$***mm*(*m..*)**
16	Ditetragonal dipyramid	Edge-truncated tetragonal prism	16	$\frac{4}{m}mm$	$\frac{\mathbf{4}}{\boldsymbol{m}}$***mm*(1)**
17	Trigonal pyramid	Trigon	3	3*m*	**3(1)**; $\left\{\begin{matrix}3m1(.m.)\\ 31m(..m)\\ 3m\ \ (.m)\end{matrix}\right.$

Table 3.2.1.3 (continued)

No.	Crystal form	Point form	Number of faces or points	Eigensymmetry	Generating point groups with oriented face (site) symmetries between parentheses
18	Trigonal prism	Trigon through origin	3	$\bar{6}2m$	3(1); $\left\{\begin{array}{l}\mathbf{321(.2.)}\\ \mathbf{312(..2)};\\ \mathbf{32}\ \ \mathbf{(.2)}\end{array}\right.$ $\left\{\begin{array}{l}3m1(.m.)\\ 31m(..m);\\ 3m\ \ (.m)\end{array}\right.$ $\bar{\mathbf{6}}(\boldsymbol{m..})$; $\left\{\begin{array}{l}\bar{\mathbf{6}}\boldsymbol{m}\mathbf{2}(\boldsymbol{mm}\mathbf{2})\\ \bar{\mathbf{6}}\mathbf{2}\boldsymbol{m}(\boldsymbol{m}\mathbf{2}\boldsymbol{m})\end{array}\right.$
19	Trigonal trapezohedron	Twisted trigonal antiprism	6	32	$\left\{\begin{array}{l}\mathbf{321(1)}\\ \mathbf{312(1)}\\ \mathbf{32}\ \ \mathbf{(1)}\end{array}\right.$
20	Ditrigonal pyramid	Truncated trigon	6	$3m$	$\left\{\begin{array}{l}\mathbf{3}\boldsymbol{m}\mathbf{1(1)}\\ \mathbf{31}\boldsymbol{m}\mathbf{(1)}\\ \mathbf{3}\boldsymbol{m}\ \ \mathbf{(1)}\end{array}\right.$
21	Rhombohedron	Trigonal antiprism	6	$\bar{3}m$	$\bar{\mathbf{3}}\mathbf{(1)}$; $\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.$ $\left\{\begin{array}{l}\bar{\mathbf{3}}\boldsymbol{m}\mathbf{1}\boldsymbol{(.m.)}\\ \bar{\mathbf{3}}\mathbf{1}\boldsymbol{m(..m)}\\ \bar{\mathbf{3}}\boldsymbol{m}\ \boldsymbol{(.m)}\end{array}\right.$
22	Ditrigonal prism	Truncated trigon through origin	6	$\bar{6}2m$	$\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.$ $\left\{\begin{array}{l}3m1(1)\\ 31m(1);\\ 3m\ \ (1)\end{array}\right.$ $\left\{\begin{array}{l}\bar{\mathbf{6}}\boldsymbol{m}\mathbf{2}\boldsymbol{(m..)}\\ \bar{\mathbf{6}}\mathbf{2}\boldsymbol{m(m..)}\end{array}\right.$
23	Hexagonal pyramid	Hexagon	6	$6mm$	$\left\{\begin{array}{l}3m1(1)\\ 31m(1);\\ 3m\ \ (1)\end{array}\right.$ $\mathbf{6(1)}$; $\boldsymbol{\mathbf{6mm}(..m,.m.)}$
24	Trigonal dipyramid	Trigonal prism	6	$\bar{6}2m$	$\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.$ $\bar{\mathbf{6}}\mathbf{(1)}$; $\left\{\begin{array}{l}\bar{\mathbf{6}}\boldsymbol{m}\mathbf{2}\boldsymbol{(.m.)}\\ \bar{\mathbf{6}}\mathbf{2}\boldsymbol{m(..m)}\end{array}\right.$
25	Hexagonal prism	Hexagon through origin	6	$\frac{6}{m}mm$	$\bar{3}(1)$; $\left\{\begin{array}{l}321(1)\\ 312(1);\\ 32\ \ (1)\end{array}\right.$ $\left\{\begin{array}{l}3m1(1)\\ 31m(1);\\ 3m\ \ (1)\end{array}\right.$ ‡$\left\{\begin{array}{l}\bar{\mathbf{3}}\boldsymbol{m}\mathbf{1}\boldsymbol{(.2.)}\ \text{and}\ \bar{3}m1(.m.)\\ \bar{\mathbf{3}}\mathbf{1}\boldsymbol{m(..2)}\ \text{and}\ \bar{3}1m(..m);\\ \bar{\mathbf{3}}\boldsymbol{m}\boldsymbol{(.2)}\ \text{and}\ \bar{3}m(.m)\end{array}\right.$ 6(1); $\frac{\mathbf{6}}{\boldsymbol{m}}\boldsymbol{(m..)}$; $\boldsymbol{\mathbf{622}(.2.,..2)}$; $6mm(..m,.m.)$; $\left\{\begin{array}{l}\bar{6}m2(m..)\\ \bar{6}2m(m..)\end{array}\right.$; $\frac{\mathbf{6}}{\boldsymbol{m}}\boldsymbol{mm(m2m,mm2)}$
26	Ditrigonal scalenohedron or hexagonal scalenohedron	Trigonal antiprism sliced off by pinacoid	12	$\bar{3}m$	$\left\{\begin{array}{l}\bar{\mathbf{3}}\boldsymbol{m}\mathbf{1(1)}\\ \bar{\mathbf{3}}\mathbf{1}\boldsymbol{m}\mathbf{(1)}\\ \bar{\mathbf{3}}\boldsymbol{m}\ \ \mathbf{(1)}\end{array}\right.$
27	Hexagonal trapezohedron	Twisted hexagonal antiprism	12	622	$\mathbf{622(1)}$
28	Dihexagonal pyramid	Truncated hexagon	12	$6mm$	$\boldsymbol{\mathbf{6mm}(\mathbf{1})}$
29	Ditrigonal dipyramid	Edge-truncated trigonal prism	12	$\bar{6}2m$	$\left\{\begin{array}{l}\bar{\mathbf{6}}\boldsymbol{m}\mathbf{2(1)}\\ \bar{\mathbf{6}}\mathbf{2}\boldsymbol{m}\mathbf{(1)}\end{array}\right.$
30	Dihexagonal prism	Truncated hexagon	12	$\frac{6}{m}mm$	$\left\{\begin{array}{l}\bar{3}m1(1)\\ \bar{3}1m(1);\\ \bar{3}m\ \ (1)\end{array}\right.$ 622(1); $6mm(1)$; $\frac{\mathbf{6}}{\boldsymbol{m}}\boldsymbol{\mathbf{mm}(m..)}$
31	Hexagonal dipyramid	Hexagonal prism	12	$\frac{6}{m}mm$	$\left\{\begin{array}{l}\bar{3}m1(1)\\ \bar{3}1m(1);\\ \bar{3}m\ \ (1)\end{array}\right.$ $\frac{6}{m}(1)$; 622(1)†; $\left\{\begin{array}{l}\bar{6}m2(1)\\ \bar{6}2m(1);\end{array}\right.$ $\frac{\mathbf{6}}{\boldsymbol{m}}\boldsymbol{\mathbf{mm}(..m,.m.)}$

Table 3.2.1.3 (continued)

No.	Crystal form	Point form	Number of faces or points	Eigensymmetry	Generating point groups with oriented face (site) symmetries between parentheses
32	Dihexagonal dipyramid	Edge-truncated hexagonal prism	24	$\frac{6}{m}mm$	$\frac{\mathbf{6}}{\boldsymbol{m}}\boldsymbol{mm}(\mathbf{1})$
33	Tetrahedron	Tetrahedron	4	$\bar{4}3m$	**23(.3.)**; $\bar{\mathbf{4}}\mathbf{3}\boldsymbol{m}(\mathbf{.3}\boldsymbol{m})$
34	Cube or hexahedron	Octahedron	6	$m\bar{3}m$	**23(2..)**; $\boldsymbol{m}\bar{\mathbf{3}}(\mathbf{2}\boldsymbol{mm}\mathbf{..})$; **432(4..)**; $\bar{\mathbf{4}}\mathbf{3}\boldsymbol{m}(\mathbf{2.}\boldsymbol{mm})$; $\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}(\mathbf{4}\boldsymbol{m}\mathbf{.}\boldsymbol{m})$
35	Octahedron	Cube	8	$m\bar{3}m$	$\boldsymbol{m}\bar{\mathbf{3}}(\mathbf{.3.})$; **432(.3.)**; $\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}(\mathbf{.3}\boldsymbol{m})$
36	Pentagon-tritetrahedron or tetartoid or tetrahedral pentagon-dodecahedron	Snub tetrahedron (= pentagon-tritetrahedron + two tetrahedra)	12	23	**23(1)**
37	Pentagon-dodecahedron or dihexahedron or pyritohedron	Irregular icosahedron (= pentagon-dodecahedron + octahedron)	12	$m\bar{3}$	23(1); $\boldsymbol{m}\bar{\mathbf{3}}(\boldsymbol{m}\mathbf{..})$
38	Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron	Cube and two tetrahedra	12	$\bar{4}3m$	23(1); $\bar{\mathbf{4}}\mathbf{3}\boldsymbol{m}(\mathbf{..}\boldsymbol{m})$
39	Trigon-tritetrahedron or tristetrahedron	Tetrahedron truncated by tetrahedron	12	$\bar{4}3m$	23(1); $\bar{\mathbf{4}}\mathbf{3}\boldsymbol{m}(\mathbf{..}\boldsymbol{m})$
40	Rhomb-dodecahedron	Cuboctahedron	12	$m\bar{3}m$	23(1); $m\bar{3}(m..)$; **432(..2)**; $\bar{4}3m(..m)$; $\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}(\boldsymbol{m}\mathbf{.}\boldsymbol{m}\mathbf{2})$
41	Didodecahedron or diploid or dyakisdodecahedron	Cube & octahedron & pentagon-dodecahedron	24	$m\bar{3}$	$\boldsymbol{m}\bar{\mathbf{3}}(\mathbf{1})$
42	Trigon-trioctahedron or trisoctahedron	Cube truncated by octahedron	24	$m\bar{3}m$	$m\bar{3}(1)$; 432(1); $\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}(\mathbf{..}\boldsymbol{m})$
43	Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron	Cube & octahedron & rhomb-dodecahedron	24	$m\bar{3}m$	$m\bar{3}(1)$; 432(1); $\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}(\mathbf{..}\boldsymbol{m})$
44	Pentagon-trioctahedron or gyroid	Cube + octahedron + pentagon-trioctahedron	24	432	**432(1)**
45	Hexatetrahedron or hexakistetrahedron	Cube truncated by two tetrahedra	24	$\bar{4}3m$	$\bar{\mathbf{4}}\mathbf{3}\boldsymbol{m}(\mathbf{1})$
46	Tetrahexahedron or tetrakishexahedron	Octahedron truncated by cube	24	$m\bar{3}m$	432(1); $\bar{4}3m(1)$; $\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}(\boldsymbol{m}\mathbf{..})$
47	Hexaoctahedron or hexakisoctahedron	Cube truncated by octahedron and by rhomb-dodecahedron	48	$m\bar{3}m$	$\boldsymbol{m}\bar{\mathbf{3}}\boldsymbol{m}(\mathbf{1})$

† These limiting forms occur in three or two non-equivalent orientations (different types of limiting forms); *cf.* Table 3.2.3.2. ‡ In point groups $\bar{4}2m$ and $\bar{3}m$, the tetragonal prism and the hexagonal prism occur twice, as a 'basic special form' and as a 'limiting special form'. In these cases, the point groups are listed twice, as '$\bar{\mathbf{4}}\mathbf{2}\boldsymbol{m}$**(.2.)** and $\bar{4}2m(..m)$' and as '$\bar{\mathbf{3}}\boldsymbol{m}$**1(.2.)** and $\bar{3}m1(.m.)$'.

hedry $6/mmm$ has to be taken). Different types of limiting forms may have the same eigensymmetry and the same topology, as shown by the examples below. The occurrence of two topologically different polyhedra as two 'realizations' of one type of limiting form in point groups 23, $m\bar{3}$ and 432 is explained below in Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).

Examples

(1) In point group 32, the limiting general crystal forms are of four types:
   (i) ditrigonal prisms, eigensymmetry $\bar{6}2m$ (face poles on horizontal mirror plane of holohedry $6/mmm$);
   (ii) trigonal dipyramids, eigensymmetry $\bar{6}2m$ (face poles on one kind of vertical mirror plane);
   (iii) rhombohedra, eigensymmetry $\bar{3}m$ (face poles on second kind of vertical mirror plane);
   (iv) hexagonal prisms, eigensymmetry $6/mmm$ (face poles on horizontal twofold axes).

   Types (i) and (ii) have the same eigensymmetry but different topologies; types (i) and (iv) have the same topology but different eigensymmetries; type (iii) differs from the other three types in both eigensymmetry and topology.

(2) In point group 222, the face poles of the three types of general limiting forms, rhombic prisms, are located on the three (non-equivalent) symmetry planes of the holohedry *mmm*. Geometrically, the axes of the prisms are directed along the three non-equivalent orthorhombic symmetry directions. The three types of limiting forms have the same

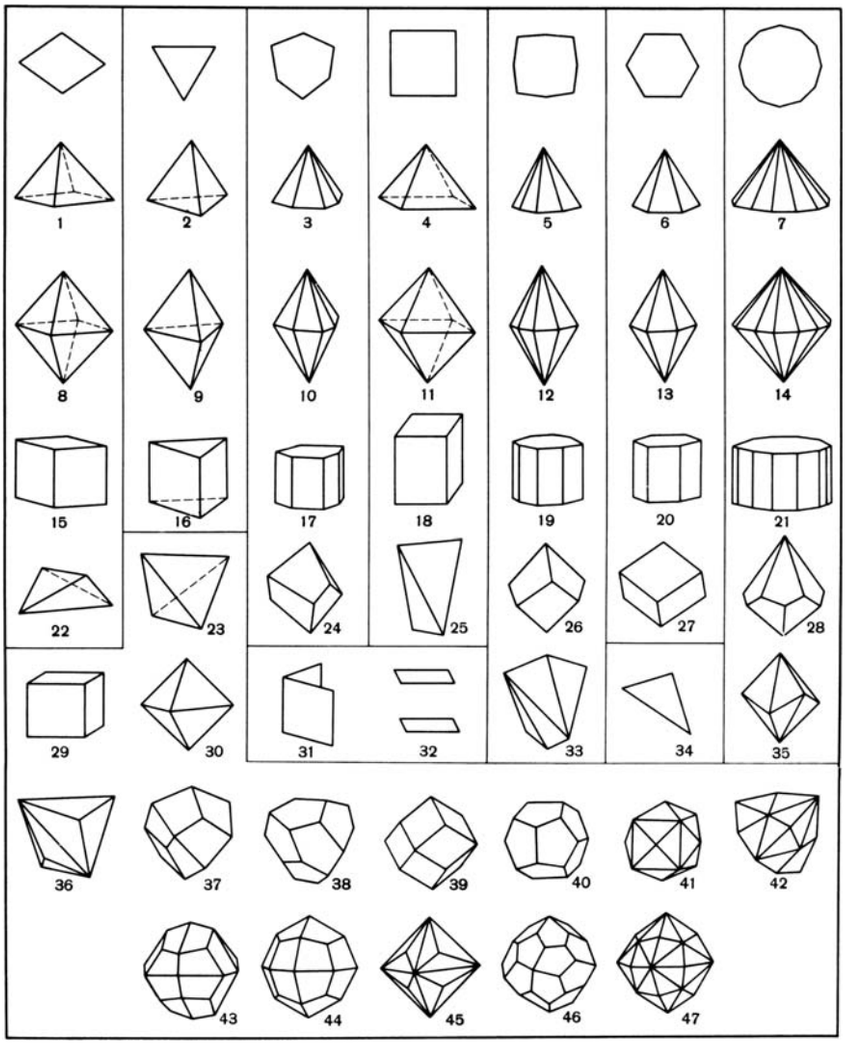


Figure 3.2.1.1
The 47 crystal forms that crystals may take (from Shubnikov & Koptsik, 1974, p. 74): (1)–(7) Pyramids: orthorhombic, trigonal, ditrigonal, tetragonal, ditetragonal, hexagonal, dihexagonal; (8)–(14) bipyramids of the same types; (15)–(21) prisms of the same types; (22), (23), (25) tetrahedra: orthorhombic, regular and tetragonal; (24), (26), (28) trapezohedra: trigonal, tetragonal, hexagonal: (27) rhombohedron; (34) scalene triangle; (33), (35) scalenohedra: tetragonal and ditrigonal; (31) dihedron (axial or non-axial); (32) pinacoid; (23), (29), (30), (36)–(47) simple forms of the cubic system: (23) tetrahedron; (29) hexahedron (cube); (30) octahedron; (36) trigonal tristetrahedron; (37) tetragonal tristetrahedron; (38) pentagonal tristetrahedron; (39) rhombic dodecahedron; (40) pentagonal dodecahedron; (41) tetrahexahedron; (42) hexatetrahedron; (43) didodecahedron; (44) tetragonal trisoctahedron; (45) trigonal trisoctahedron; (46) pentagonal trisoctahedron; (47) hexoctahedron. The central cross sections of all the figures above the stepped line dividing the table are the regular polygons indicated in the top row. Note that the numbers in this figure do not correspond to the numbers used in column 1 of Table 3.2.1.3.

eigensymmetry and the same topology but different orientations.

Similar cases occur in point groups 422 and 622 (*cf.* the first footnote to Table 3.2.1.3).

Not considered in this volume are limiting forms of another kind, namely those that require either special metrical conditions for the axial ratios or irrational indices or coordinates (which always can be closely approximated by rational values). For instance, a rhombic disphenoid can, for special axial ratios, appear as a tetragonal or even as a cubic tetrahedron; similarly, a rhombohedron can degenerate to a cube. For special irrational indices, a ditetragonal prism changes to a (noncrystallographic) octagonal prism, a dihexagonal pyramid to a dodecagonal pyramid or a crystallographic pentagon-dodecahedron to a regular pentagon-dodecahedron. These kinds of limiting forms are listed by A. Niggli (1963).

In conclusion, each general or special Wyckoff position always contains one set of basic crystal (point) forms. In addition, it may contain one or more sets of limiting forms of different types. As a rule,[7] each type comprises polyhedra of the same eigensymmetry and topology and, hence, of the same name, for instance 'ditetragonal pyramid'. The name of the *basic general* forms is often used to designate the corresponding crystal class, for instance 'ditetragonal-pyramidal class'; some of these names are listed in Table 3.2.1.4.

3.2.1.2.3. Description of crystal and point forms

The main part of each point-group table in Section 3.2.3 describes the general and special *crystal and point forms* of that point group, in a manner analogous to the *positions* in a space group. The general Wyckoff position is given at the top, followed downwards by the special Wyckoff positions with decreasing multiplicity. Within each Wyckoff position, the first block of column 6 refers to the basic forms, the subsequent blocks list the various types of limiting form, if any.

The columns, from left to right, contain the following data (further details are to be found below in Section 3.2.1.2.4, *Notes on crystal and point forms*):

Column 1: *Multiplicity* of the 'Wyckoff position', *i.e.* the number of equivalent faces and points of a crystal or point form.

Column 2: *Wyckoff letter.* Each general or special 'Wyckoff position' is designated by a 'Wyckoff letter', analogous to the Wyckoff letter of a position in a space group (*cf.* Sections 1.4.4.2 and 2.1.3.11).

Column 3: *Face symmetry* or *site symmetry*, given in the form of an 'oriented point-group symbol', analogous to the oriented site-symmetry symbols of space groups (*cf.* Sections 1.4.4.2 and 2.1.3.12). The face symmetry is also the symmetry of etch pits, striations and other face markings. For the two-dimensional point groups, this column contains the *edge symmetry*, which can be either 1 or *m*.

Column 4: *Coordinates* x, y, z of the symmetry-equivalent points of a point form.

Column 5: *Name of crystal form.* If more than one name is in common use, several are listed. The names of the limiting forms are also given. The crystal forms, their names, eigensymmetries and occurrence in the point groups are summarized in Table 3.2.1.3, which may be useful for determinative purposes, as explained in Sections 3.2.2.2 and 3.2.2.3. There are 47 different

[7] For the exceptions in the cubic crystal system *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).

Table 3.2.1.4
Names and symbols of the 32 crystal classes

System used in this volume	Point group: International symbol: Short	Point group: International symbol: Full	Schoenflies symbol	Class names: Groth (1921)	Class names: Friedel (1926)	
Triclinic	1	1	C_1	Pedial (asymmetric)	Hemihedry	
	$\overline{1}$	$\overline{1}$	$C_i(S_2)$	Pinacoidal	Holohedry	
Monoclinic	2	2	C_2	Sphenoidal	Holoaxial hemihedry	
	m	m	$C_s(C_{1h})$	Domatic	Antihemihedry	
	$2/m$	$\frac{2}{m}$	C_{2h}	Prismatic	Holohedry	
Orthorhombic	222	222	$D_2(V)$	Disphenoidal	Holoaxial hemihedry	
	$mm2$	$mm2$	C_{2v}	Pyramidal	Antihemihedry	
	mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_{2h}(V_h)$	Dipyramidal	Holohedry	
Tetragonal	4	4	C_4	Pyramidal	Tetartohedry with 4-axis	
	$\overline{4}$	$\overline{4}$	S_4	Disphenoidal	Sphenohedral tetartohedry	
	$4/m$	$\frac{4}{m}$	C_{4h}	Dipyramidal	Parahemihedry	
	422	422	D_4	Trapezohedral	Holoaxial hemihedry	
	$4mm$	$4mm$	C_{4v}	Ditetragonal-pyramidal	Antihemihedry with 4-axis	
	$\overline{4}2m$	$\overline{4}2m$	$D_{2d}(V_d)$	Scalenohedral	Sphenohedral antihemihedry	
	$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	D_{4h}	Ditetragonal-dipyramidal	Holohedry	
					Hexagonal	*Rhombohedral*
Trigonal	3	3	C_3	Pyramidal	Ogdohedry	Tetartohedry
	$\overline{3}$	$\overline{3}$	$C_{3i}(S_6)$	Rhombohedral	Paratetartohedry	Parahemihedry
	32	32	D_3	Trapezohedral	Holoaxial tetartohedry with 3-axis	Holoaxial hemihedry
	$3m$	$3m$	C_{3v}	Ditrigonal-pyramidal	Hemimorphic antitetartohedry	Antihemihedry
	$\overline{3}m$	$\overline{3}\frac{2}{m}$	D_{3d}	Ditrigonal-scalenohedral	Parahemihedry with 3-axis	Holohedry
Hexagonal	6	6	C_6	Pyramidal	Tetartohedry with 6-axis	
	$\overline{6}$	$\overline{6}$	C_{3h}	Trigonal-dipyramidal	Trigonohedral antitetartohedry	
	$6/m$	$\frac{6}{m}$	C_{6h}	Dipyramidal	Parahemihedry with 6-axis	
	622	622	D_6	Trapezohedral	Holoaxial hemihedry	
	$6mm$	$6mm$	C_{6v}	Dihexagonal-pyramidal	Antihemihedry with 6-axis	
	$\overline{6}2m$	$\overline{6}2m$	D_{3h}	Ditrigonal-dipyramidal	Trigonohedral antihemihedry	
	$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	D_{6h}	Dihexagonal-dipyramidal	Holohedry	
Cubic	23	23	T	Tetrahedral-pentagondodecahedral (= tetartoidal)	Tetartohedry	
	$m\overline{3}$	$\frac{2}{m}\overline{3}$	T_h	Disdodecahedral (= diploidal)	Parahemihedry	
	432	432	O	Pentagon-icositetrahedral (= gyroidal)	Holoaxial hemihedry	
	$\overline{4}3m$	$\overline{4}3m$	T_d	Hexakistetrahedral (= hextetrahedral)	Antihemihedry	
	$m\overline{3}m$	$\frac{4}{m}\overline{3}\frac{2}{m}$	O_h	Hexakisoctahedral (= hexoctahedral)	Holohedry	

types of crystal form. Frequently, 48 are quoted because 'sphenoid' and 'dome' are considered as two different forms. It is customary, however, to regard them as the same form, with the name 'dihedron'.

Name of point form (printed in italics). There exists no general convention on the names of the point forms. Here, only one name is given, which does not always agree with that of other authors. The names of the point forms are also contained in Table 3.2.1.3. Note that the same point form, 'line segment', corresponds to both sphenoid and dome.

Column 6: *Miller indices* (*hkl*) for the symmetry-equivalent faces (edges) of a crystal form. In the trigonal and hexagonal crystal systems, when referring to hexagonal axes, Bravais–Miller indices (*hkil*) are used, with $h + k + i = 0$.

With a few exceptions, the triplets of Miller indices (*hkl*) and point coordinates x, y, z are arranged in such a way as to show

analogous sequences; they are both based on the same set of generators, as described in Sections 1.4.3 and 2.1.3.10. For all point groups, except those referred to a hexagonal coordinate system, the correspondence between the (hkl) and the x, y, z triplets is immediately obvious.[8]

The sets of symmetry-equivalent crystal faces also represent the sets of equivalent reciprocal-lattice points, as well as the sets of equivalent X-ray (neutron) reflections. This important aspect is treated in Klapper & Hahn (2010).

Examples

(1) In point group $\overline{4}$, the general crystal form 4*b* is listed as (hkl) $(\overline{h}\,\overline{k}l)$ $(k\overline{h}\,\overline{l})$ $(\overline{k}h\overline{l})$: the corresponding general position 4*h* of the symmorphic space group $P\overline{4}$ reads x, y, z; $\overline{x}, \overline{y}, z$; $y, \overline{x}, \overline{z}$; $\overline{y}, x, \overline{z}$.

(2) In point group 3 (hexagonal axes), the general crystal form 3*b* is listed as $(hkil)$ $(ihkl)$ $(kihl)$ with $i = -(h + k)$; the corresponding general point form 3*b* is x, y, z; $\overline{y}, x - y, z$; $\overline{x} + y, \overline{x}, z$.

(3) The Miller indices of the *cubic point groups* are arranged in one, two or four blocks of (3×4) entries. The first block belongs to point group 23. The second block belongs to the diagonal twofold axes in 432 and $m\overline{3}m$ or to the diagonal mirror plane in $\overline{4}3m$. In point groups $m\overline{3}$ and $m\overline{3}m$, the lower one or two blocks are derived from the upper blocks by application of the inversion.

Further discussion of the data in Tables 3.2.3.1 and 3.2.3.2 as far as molecular symmetry is concerned can be found in Section 3.2.4.3.

3.2.1.2.4. Notes on crystal and point forms

(i) As mentioned in Section 3.2.1.1, each set of Miller indices of a given point group represents infinitely many face forms with the same name. Exceptions occur for the following cases.

Some special crystal forms occur with only *one* representative. Examples are the pinacoid {001}, the hexagonal prism $\{10\overline{1}0\}$ and the cube {100}. The Miller indices of these forms consist of fixed numbers and signs and contain no variables.

In a few noncentrosymmetric point groups, a special crystal form is realized by *two* representatives: they are related by a centre of symmetry that is not part of the point-group symmetry. These cases are

(*a*) the two opposite, polar pedions (001) and $(00\overline{1})$;

(*b*) the two trigonal prisms $\{10\overline{1}0\}$ and $\{\overline{1}010\}$; similarly for two dimensions;

(*c*) the two trigonal prisms $\{11\overline{2}0\}$ and $\{\overline{1}\,\overline{1}20\}$; similarly for two dimensions;

(*d*) the positive and negative tetrahedra {111} and $\{\overline{1}\,\overline{1}\,\overline{1}\}$.

In the point-group tables, both representatives of these forms are listed, separated by 'or', for instance '(001) or $(00\overline{1})$'.

(ii) In crystallography, the terms tetragonal, trigonal, hexagonal, as well as tetragon, trigon and hexagon, imply that the cross sections of the corresponding polyhedra, or the polygons, are *regular* tetragons (squares), trigons or hexagons. Similarly, ditetragonal, ditrigonal, dihexagonal, as well as ditetragon, ditrigon and dihexagon, refer to *semi-regular* cross sections or polygons.

(iii) Crystal forms can be 'open' or 'closed'. A crystal form is 'closed' if its faces form a closed polyhedron; the minimum number of faces for a closed form is 4. Closed forms are disphenoids, dipyramids, rhombohedra, trapezohedra, scalenohedra and all cubic forms; open forms are pedions, pinacoids, sphenoids (domes), pyramids and prisms.

A point form is always closed. It should be noted, however, that a point form dual to a *closed* face form is a *three*-dimensional polyhedron, whereas the dual of an *open* face form is a *two*- or *one*-dimensional polygon, which, in general, is located 'off the origin' but may be centred at the origin (here called 'through the origin').

(iv) Crystal forms are well known; they are described and illustrated in many textbooks. Crystal forms are 'isohedral' polyhedra that have all faces equivalent but may have more than one kind of vertex; they include regular polyhedra. The in-sphere of the polyhedron touches all the faces.

Crystallographic point forms are less known; they are described in a few places only, notably by A. Niggli (1963), by Fischer *et al.* (1973), and by Burzlaff & Zimmermann (1977). The latter publication contains drawings of the polyhedra of all point forms. Point forms are 'isogonal' polyhedra (polygons) that have all vertices equivalent but may have more than one kind of face;[9] again, they include regular polyhedra. The circumsphere of the polyhedron passes through all the vertices.

In most cases, the names of the point-form polyhedra can easily be derived from the corresponding crystal forms: the duals of *n*-gonal pyramids are regular *n*-gons off the origin, those of *n*-gonal prisms are regular *n*-gons through the origin. The duals of di-*n*-gonal pyramids and prisms are truncated (regular) *n*-gons, whereas the duals of *n*-gonal dipyramids are *n*-gonal prisms.

In a few cases, however, the relations are not so evident. This applies mainly to some cubic point forms [see item (v) below]. A further example is the rhombohedron, whose dual is a trigonal antiprism (in general, the duals of *n*-gonal streptohedra are *n*-gonal antiprisms).[10] The duals of *n*-gonal trapezohedra are polyhedra intermediate between *n*-gonal prisms and *n*-gonal antiprisms; they are called here 'twisted *n*-gonal antiprisms' (example: point group 622). Finally, the duals of di-*n*-gonal scalenohedra are *n*-gonal antiprisms 'sliced off' perpendicular to the prism axis by the pinacoid {001}.[11]

(v) Some cubic point forms have to be described by 'combinations' of 'isohedral' polyhedra because no common

[8] The matrices of corresponding triplets $(\tilde{h}\tilde{k}\tilde{l})$ and $\tilde{x}, \tilde{y}, \tilde{z}$, *i.e.* of triplets generated by the same symmetry operation from (hkl) and x, y, z, are inverse to each other, provided the x, y, z and $\tilde{x}, \tilde{y}, \tilde{z}$ are regarded as columns and the (hkl) and $(\tilde{h}\tilde{k}\tilde{l})$ as rows: this is due to the contravariant and covariant nature of the point coordinates and Miller indices, respectively. Note that for orthogonal matrices the inverse matrix equals the transposed matrix; in crystallography, this applies to all coordinate systems (including the rhombohedral one), except for the hexagonal system. The matrices for the symmetry operations occurring in the crystallographic point groups are listed in Tables 1.2.2.1 and 1.2.2.2.

[9] Thus, the name 'prism' for a *point form* implies combination of the prism with a pinacoid.

[10] A tetragonal tetrahedron is a digonal streptohedron; hence, its dual is a 'digonal antiprism', which is again a tetragonal tetrahedron.

[11] The dual of a tetragonal (= di-digonal) scalenohedron is a 'digonal antiprism', which is 'cut off' by the pinacoid {001}.

names exist for 'isogonal' polyhedra. The maximal number of polyhedra required is three. The *shape* of the combination that describes the point form depends on the relative sizes of the polyhedra involved, *i.e.* on the relative values of their central distances. Moreover, in some cases even the *topology* of the point form may change.

Example

'Cube truncated by octahedron' and 'octahedron truncated by cube'. Both forms have 24 vertices, 14 faces and 36 edges, but the faces of the first combination are octagons and trigons, those of the second are hexagons and tetragons. These combinations represent different special point forms x, y, z and $0, y, z$. One form can change into the other only *via* the (semi-regular) cuboctahedron $0, y, y$, which has 12 vertices, 14 faces and 24 edges.

The unambiguous description of the cubic point forms by combinations of 'isohedral' polyhedra requires restrictions on the relative sizes of the polyhedra of a combination. The permissible range of the size ratios is limited on the one hand by vanishing, on the other hand by splitting of vertices of the combination. Three cases have to be distinguished:

(a) The relative sizes of the polyhedra of the combination can vary *independently.* This occurs whenever three edges meet in one vertex. In Table 3.2.3.2, the names of these point forms contain the term 'truncated'.

Examples

(1) 'Octahedron truncated by cube' (24 vertices, dual to tetrahexahedron).

(2) 'Cube truncated by two tetrahedra' (24 vertices, dual to hexatetrahedron), implying independent variation of the relative sizes of the two truncating tetrahedra.

(b) The relative sizes of the polyhedra are *interdependent.* This occurs for combinations of three polyhedra whenever four edges meet in one vertex. The names of these point forms contain the symbol '&'.

Example

'Cube & two tetrahedra' (12 vertices, dual to tetragon-tritetrahedron); here the interdependence results from the requirement that in the combination a cube edge is reduced to a vertex in which faces of the two tetrahedra meet. The location of this vertex on the cube edge is free. A higher-symmetry 'limiting' case of this combination is the 'cuboctahedron', where the two tetrahedra have the same sizes and thus form an octahedron.

(c) The relative sizes of the polyhedra are *fixed.* This occurs for combinations of three polyhedra if five edges meet in one vertex. These point forms are designated by special names (snub tetrahedron, snub cube, irregular icosahedron), or their names contain the symbol '+'.

The cuboctahedron appears here too, as a limiting form of the snub tetrahedron (dual to pentagon-tritetrahedron) and of the irregular icosahedron (dual to pentagon-dodecahedron) for the special coordinates $0, y, y$.

(vi) Limiting crystal forms result from general or special crystal forms for special values of certain geometrical parameters of the form.

Examples

(1) A pyramid degenerates into a prism if its apex angle becomes 0, *i.e.* if the apex moves towards infinity.

(2) In point group 32, the general form is a trigonal trapezohedron $\{hkl\}$; this form can be considered as two opposite trigonal pyramids, rotated with respect to each other by an angle χ. The trapezohedron changes into the limiting forms 'trigonal dipyramid' $\{hhl\}$ for $\chi = 0^\circ$ and 'rhombohedron' $\{h0l\}$ for $\chi = 60^\circ$.

(vii) One and the same type of polyhedron can occur as a general, special or limiting form.

Examples

(1) A tetragonal dipyramid is a general form in point group $4/m$, a special form in point group $4/mmm$ and a limiting general form in point groups 422 and $\overline{4}2m$.

(2) A tetragonal prism appears in point group $\overline{4}2m$ both as a basic special form ($4b$) and as a limiting special form ($4c$).

(viii) A peculiarity occurs for the cubic point groups. Here the crystal forms $\{hhl\}$ are realized as two topologically different kinds of polyhedra with the same face symmetry, multiplicity and, in addition, the same eigensymmetry. The realization of one or other of these forms depends upon whether the Miller indices obey the conditions $|h| > |l|$ or $|h| < |l|$, *i.e.* whether, in the stereographic projection, a face pole is located between the directions [110] and [111] or between the directions [111] and [001]. These two kinds of polyhedra have to be considered as two *realizations* of *one type* of crystal form because their face poles are located on the same set of conjugate symmetry elements. Similar considerations apply to the point forms x, x, z.

In the point groups $m\overline{3}m$ and $\overline{4}3m$, the two kinds of polyhedra represent two realizations of one *special* 'Wyckoff position'; hence, they have the same Wyckoff letter. In the groups 23, $m\overline{3}$ and 432, they represent two realizations of the same type of limiting *general* forms. In the tables of the cubic point groups, the two entries are always connected by braces.

The same kind of peculiarity occurs for the two icosahedral point groups, as mentioned in Section 3.2.1.4.2 and listed in Table 3.2.2.1.

3.2.1.2.5. Names and symbols of the crystal classes

Several different sets of names have been devised for the 32 crystal classes. Their use, however, has greatly declined since the introduction of the international point-group symbols. As examples, two sets (both translated into English) that are frequently found in the literature are given in Table 3.2.1.4. To the name of the class the name of the system has to be added: *e.g.* 'tetragonal pyramidal' or 'tetragonal tetartohedry'.

Note that Friedel (1926) based his nomenclature on the point symmetry of the lattice. Hence, two names are given for the five trigonal point groups, depending whether the lattice is hexagonal

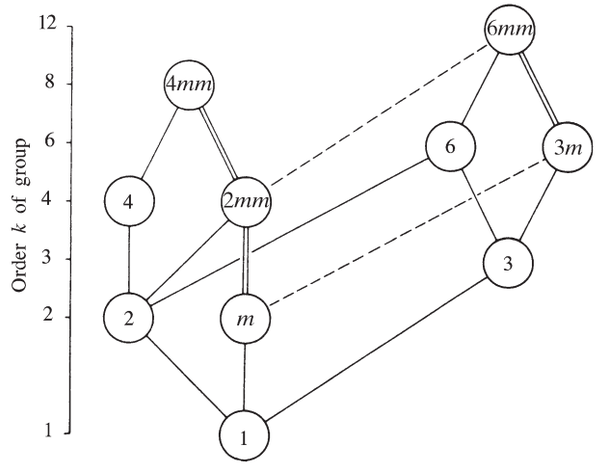


Figure 3.2.1.2
Maximal subgroups and minimal supergroups of the two-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left.

or rhombohedral: *e.g.* 'hexagonal ogdohedry' and 'rhombohedral tetartohedry'.

3.2.1.3. Subgroups and supergroups of the crystallographic point groups

In this section, the sub- and supergroup relations between the crystallographic point groups are presented in the form of a 'family tree'.[12] Figs. 3.2.1.2 and 3.2.1.3 apply to two and three dimensions. The sub- and supergroup relations between two groups are represented by solid or dashed lines. For a given point group $\mathcal{P}$ of order k_P the lines to groups of lower order connect $\mathcal{P}$ with all its *maximal subgroups* $\mathcal{H}$ with orders k_H; the index $[i]$ of each subgroup is given by the ratio of the orders k_P/k_H. The lines to groups of higher order connect $\mathcal{P}$ with all its *minimal supergroups* $\mathcal{S}$ with orders k_S; the index $[i]$ of each supergroup is given by the ratio k_S/k_P. In other words: if the diagram is read downwards, subgroup relations are displayed; if it is read upwards, supergroup relations are revealed. The index is always an integer (theorem of Lagrange) and can be easily obtained from the group orders given on the left of the diagrams. The highest index of a maximal subgroup is [3] for two dimensions and [4] for three dimensions.

Two important kinds of subgroups, namely sets of conjugate subgroups and normal subgroups, are distinguished by dashed and solid lines. They are characterized as follows:

The subgroups $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ of a group $\mathcal{P}$ are *conjugate* subgroups if $\mathcal{H}_1, \mathcal{H}_2, \ldots, \mathcal{H}_n$ are symmetry-equivalent in $\mathcal{P}$, *i.e.* if for every pair $\mathcal{H}_i, \mathcal{H}_j$ at least one symmetry operation W of $\mathcal{P}$ exists which maps $\mathcal{H}_i$ onto $\mathcal{H}_j$: $W^{-1}\mathcal{H}_i W = \mathcal{H}_j$; *cf.* Sections 1.1.5 and 1.1.8.

Examples

(1) Point group $3m$ has three different mirror planes which are equivalent due to the threefold axis. In each of the three maximal subgroups of type m, one of these mirror planes is retained. Hence, the three subgroups m are conjugate in $3m$. This set of conjugate subgroups is represented by *one* dashed line in Figs. 3.2.1.2 and 3.2.1.3.

(2) Similarly, group 432 has three maximal conjugate subgroups of type 422 and four maximal conjugate subgroups of type 32.

The subgroup $\mathcal{H}$ of a group $\mathcal{P}$ is a *normal* (or invariant) subgroup if *no* subgroup $\mathcal{H}'$ of $\mathcal{P}$ exists that is conjugate to $\mathcal{H}$ in $\mathcal{P}$. Note that this does not imply that $\mathcal{H}$ is also a normal subgroup of any supergroup of $\mathcal{P}$. Subgroups of index [2] are always normal and maximal (*cf.* Section 1.1.5). (The role of normal subgroups for the structure of space groups is discussed in Sections 1.3.3 and 1.4.2.3.)

Examples

(1) Fig. 3.2.1.3 shows two solid lines between point groups 422 and 222, indicating that 422 has two maximal normal subgroups 222 of index [2]. The symmetry elements of one subgroup are rotated by 45° around the c axis with respect to those of the other subgroup. Thus, in one subgroup the symmetry elements of the two secondary, in the other those of the two tertiary tetragonal symmetry directions (*cf.* Table 2.1.3.1) are retained, whereas the primary twofold axis is the same for both subgroups. There exists no symmetry operation of 422 that maps one subgroup onto the other. This is illustrated by the stereograms below. The two normal subgroups can be indicated by the 'oriented symbols' 222. and 2.22.

(2) Similarly, group 432 has one maximal normal subgroup, 23.

Figs. 3.2.1.2 and 3.2.1.3 show that there exist two 'summits' in both two and three dimensions from which all other point groups can be derived by 'chains' of maximal subgroups. These summits are formed by the square and the hexagonal holohedry in two dimensions and by the cubic and the hexagonal holohedry in three dimensions.

The sub- and supergroups of the point groups are useful both in their own right and as a basis of the *translationengleiche* or *t* subgroups and supergroups of space groups (*cf.* Section 1.7.1). Tables of the sub- and supergroups of the plane groups and space groups are contained in Volume A1 of *International Tables for Crystallography* (2010). A general discussion of sub- and supergroups of crystallographic groups, together with further explanations and examples, is given in Section 1.7.1.

3.2.1.4. Noncrystallographic point groups

3.2.1.4.1. Description of general point groups

In Sections 3.2.1.2 and 3.2.1.3, only the 32 *crystallographic* point groups (crystal classes) are considered. In addition, infinitely many *noncrystallographic* point groups exist that are of interest as possible symmetries of molecules and of quasicrystals and as approximate local site symmetries in crystals. Crystallographic *and* noncrystallographic point groups are collected here under the name *general point groups*. They are reviewed in this section and listed in Tables 3.2.1.5 and 3.2.1.6.

[12] This type of diagram was first used in *International Tables for the Determination of Crystal Structures* (1935): in *International Tables for X-ray Crystallography* (1952) a somewhat different approach was employed.

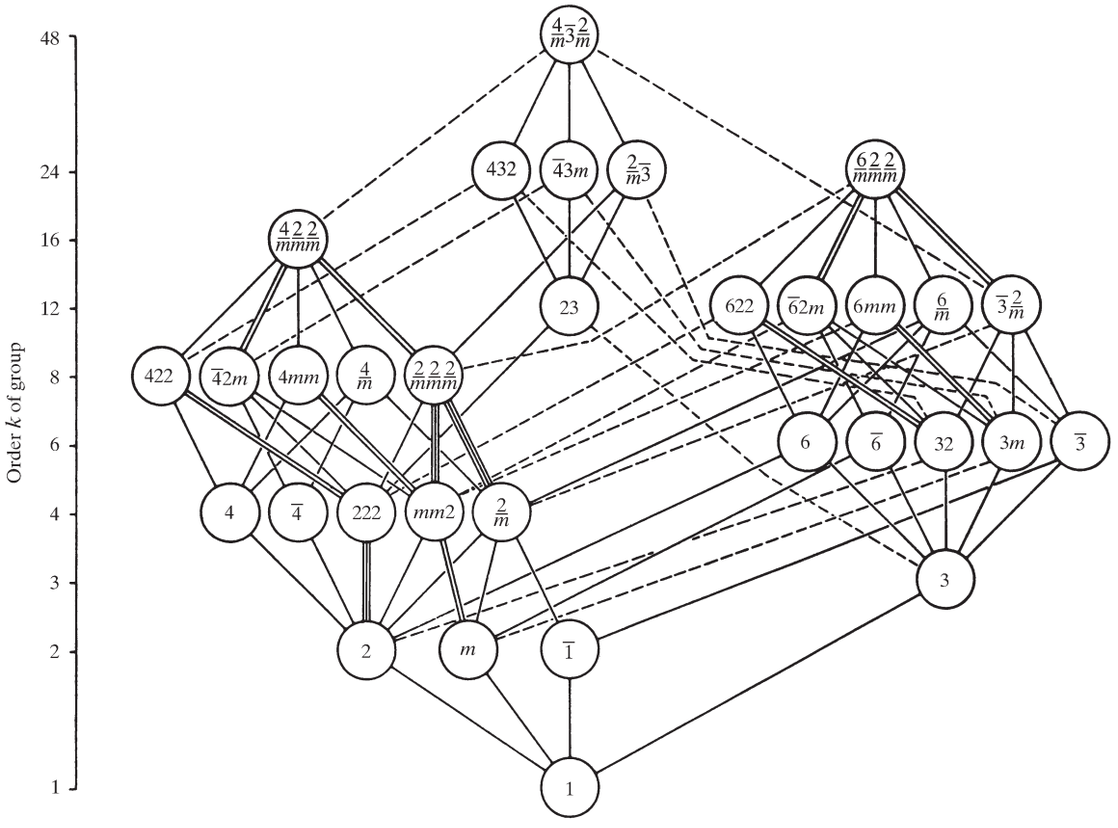


Figure 3.2.1.3
Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left. Full Hermann–Mauguin symbols are used.

Because of the infinite number of these groups only *classes of general point groups* (*general classes*)[13] can be listed. They are grouped into *general systems*, which are similar to the crystal systems. The 'general classes' are of two kinds: in the cubic, icosahedral, circular, cylindrical and spherical system, each general class contains *one* point group only, whereas in the $4N$-gonal, $(2N+1)$-gonal and $(4N+2)$-gonal system, each general class contains *infinitely* many point groups, which differ in their principal n-fold symmetry axis, with $n = 4, 8, 12, \ldots$ for the $4N$-gonal system, $n = 1, 3, 5, \ldots$ for the $(2N+1)$-gonal system and $n = 2, 6, 10, \ldots$ for the $(4N+2)$-gonal system.

Furthermore, some general point groups are of order infinity because they contain symmetry axes (rotation or rotoinversion axes) of order infinity[14] (∞-fold axes). These point groups occur in the circular system (two dimensions) and in the cylindrical and spherical systems (three dimensions).

The Hermann–Mauguin and Schoenflies symbols for the general point groups follow the rules of the crystallographic point groups (*cf.* Sections 1.4.1, 2.1.3.4 and 3.3.1). This extends also to the infinite groups where symbols like ∞m or $C_{\infty v}$ are immediately obvious.

In *two dimensions* (Table 3.2.1.5), the eight general classes are collected into three systems. Two of these, the $4N$-gonal and the $(4N+2)$-gonal systems, contain only point groups of finite order with one n-fold rotation point each. These systems are generalizations of the square and hexagonal crystal systems. The circular system consists of two infinite point groups, with one ∞-fold rotation point each.

In *three dimensions* (Table 3.2.1.6), the 33 general classes are collected into seven systems. Three of these, the $4N$-gonal, the $(2N+1)$-gonal and the $(4N+2)$-gonal systems,[15] contain only point groups of finite order with one principal n-fold symmetry axis each. These systems are generalizations of the tetragonal, trigonal and hexagonal crystal systems (*cf.* Table 3.2.3.2). The five cubic groups are well known as crystallographic groups. The two icosahedral groups of orders 60 and 120, characterized by special combinations of twofold, threefold and fivefold symmetry axes, are discussed in more detail below. The groups of the cylindrical and the spherical systems are all of order infinity; they describe the symmetries of cylinders, cones, rotation ellipsoids, spheres *etc.*[16]

[13] The 'classes of general point groups' are not the same as the commonly used 'crystal classes' because some of them contain point groups of *different orders*. All these orders, however, follow a common scheme. In this sense, the 'general classes' are an extension of the concept of (geometric) crystal classes. For example, the general class *nmm* of the $4N$-gonal system contains the point groups $4mm$ (tetragonal), $8mm$ (octagonal), $12mm$ (dodecagonal), $16mm$ *etc.*

[14] The axes of order infinity, as considered here, do not correspond to cyclic groups (as do the axes of finite order) because there is no smallest rotation from which all other rotations can be derived as higher powers, *i.e.* by successive application. Instead, rotations of all possible angles exist. Nevertheless, it is customary to symbolize these axes as ∞ or C_∞; note that the Hermann–Mauguin symbols ∞/m and $\overline{\infty}$ are equivalent, and so are the Schoenflies symbols $C_{\infty h}$, S_∞ and $C_{\infty i}$. (There exist also axes of order infinity that do correspond to cyclic groups, namely axes based upon smallest rotations with irrational values of the rotation angle.)

[15] Here, the $(2N+1)$-gonal and the $(4N+2)$-gonal systems are distinguished in order to bring out the analogy with the trigonal and the hexagonal crystal systems. They could equally well be combined into one, in correspondence with the hexagonal 'crystal family' (*cf.* Sections 1.3.4.4 and 2.1.1).

[16] The terms 'rotating' and 'stationary' in the circular, cylindrical and spherical systems do not imply any relation to dynamical properties (motions) of crystals or molecules. They only serve to illustrate the absence (group ∞) or presence (∞m, $\overline{\infty}m$) of 'vertical' mirror planes in these groups or order ∞.

Table 3.2.1.5
Classes of general point groups in two dimensions (N = integer ≥ 0)

General Hermann–Mauguin symbol	Order of group	General edge form	General point form	Crystallographic groups
$4N$-gonal system (n-fold rotation point with $n = 4N$)				
n	n	Regular n-gon	Regular n-gon	4
nmm	$2n$	Semiregular di-n-gon	Truncated n-gon	$4mm$
$(4N+2)$-gonal system (n-fold or $\frac{1}{2}n$-fold rotation point with $n = 4N+2$)				
$\frac{1}{2}n$	$\frac{1}{2}n$	Regular $\frac{1}{2}n$-gon	Regular $\frac{1}{2}n$-gon	1, 3
$\frac{1}{2}nm$	n	Semiregular di-$\frac{1}{2}n$-gon	Truncated $\frac{1}{2}n$-gon	m, $3m$
n	n	Regular n-gon	Regular n-gon	2, 6
nmm	$2n$	Semiregular di-n-gon	Truncated n-gon	$2mm$, $6mm$
Circular system†				
∞	∞	Rotating circle	Rotating circle	–
∞m	∞	Stationary circle	Stationary circle	–

† A rotating circle has no mirror lines; there exist two enantiomorphic circles with opposite senses of rotation. A stationary circle has infinitely many mirror lines through its centre.

It is possible to define the three-dimensional point groups on the basis of either rotoinversion axes $\overline{n}$ or rotoreflection axes $\tilde{n}$. The equivalence between these two descriptions is apparent from the following examples:

$$\begin{array}{lllll} n=4N: & \overline{4}=\tilde{4} & \overline{8}=\tilde{8} & \ldots & \overline{n}=\tilde{n} \\ n=2N+1: & \overline{1}=\tilde{2} & \overline{3}=\tilde{6}=3\times\overline{1} & \ldots & \overline{n}=\widetilde{2n}=n\times\overline{1} \\ n=4N+2: & \overline{2}=\tilde{1}=m & \overline{6}=\tilde{3}=3/m & \ldots & \overline{n}=\widetilde{\tfrac{1}{2}n}=\tfrac{1}{2}n/m. \end{array}$$

In the present tables, the standard convention of using rotoinversion axes is followed.

Tables 3.2.1.5 and 3.2.1.6 contain for each class its general Hermann–Mauguin and Schoenflies symbols, the group order and the names of the general face form and its dual, the general point form.[17] Special and limiting forms are not given, nor are 'Miller indices' (hkl) and point coordinates x, y, z. They can be derived easily from Tables 3.2.3.1 and 3.2.3.2 for the crystallographic groups.[18]

3.2.1.4.2. The two icosahedral groups

The two point groups 235 and $m\bar{3}\bar{5}$ of the icosahedral system (orders 60 and 120) are of particular interest among the noncrystallographic groups because of the occurrence of fivefold axes and their increasing importance as symmetries of molecules (viruses), of quasicrystals, and as approximate local site symmetries in crystals (alloys, B_{12} icosahedron). Furthermore, they contain as special forms the two noncrystallographic *platonic solids*, the regular icosahedron (20 faces, 12 vertices) and its dual, the regular pentagon-dodecahedron (12 faces, 20 vertices).

The icosahedral groups (*cf.* diagrams in Table 3.2.3.3) are characterized by six fivefold axes that include angles of 63.43°. Each fivefold axis is surrounded by five threefold and five twofold axes, with angular distances of 37.38° between a fivefold and a threefold axis and of 31.72° between a fivefold and a twofold axis. The angles between neighbouring threefold axes are 41.81°, between neighbouring twofold axes 36°. The smallest angle between a threefold and a twofold axis is 20.90°.

Each of the six fivefold axes is perpendicular to five twofold axes; there are thus six maximal conjugate pentagonal subgroups of types 52 (for 235) and $\overline{5}m$ (for $m\bar{3}\bar{5}$) with index [6]. Each of the ten threefold axes is perpendicular to three twofold axes, leading to ten maximal conjugate trigonal subgroups of types 32 (for 235) and $\overline{3}m$ (for $m\bar{3}\bar{5}$) with index [10]. There occur, furthermore, five maximal conjugate cubic subgroups of types 23 (for 235) and $m\overline{3}$ (for $m\bar{3}\bar{5}$) with index [5].

The two icosahedral groups are listed in Table 3.2.3.3, in a form similar to the cubic point groups in Table 3.2.3.2. Each group is illustrated by stereographic projections of the symmetry elements and the general face poles (general points); the complete sets of symmetry elements are listed below the stereograms. Both groups are referred to a cubic coordinate system, with the coordinate axes along three twofold rotation axes and with four threefold axes along the body diagonals. This relation is well brought out by symbolizing these groups as 235 and $m\bar{3}\bar{5}$ instead of the customary symbols 532 and $\bar{5}\bar{3}m$.

The table contains also the multiplicities, the Wyckoff letters and the names of the general and special face forms and their duals, the point forms, as well as the oriented face- and site-symmetry symbols. In the icosahedral 'holohedry' $m\bar{3}\bar{5}$, the *special* 'Wyckoff position' 60*d* occurs in three realizations, *i.e.* with three types of polyhedra. In 235, however, these three types of polyhedra are different realizations of the limiting *general* forms, which depend on the location of the poles with respect to the axes 2, 3 and 5. For this reason, the three entries are connected by braces; *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms*, item (viii).

Not included are the sets of equivalent Miller indices and point coordinates. Instead, only the 'initial' triplets (hkl) and x, y, z for each type of form are listed. The complete sets of indices and coordinates can be obtained in two steps[19] as follows:

[17] The noncrystallographic face and point forms are extensions of the corresponding crystallographic forms: *cf.* Section 3.2.1.2.4, *Notes on crystal and point forms.* The name *streptohedron* applies to the general face forms of point groups $\overline{n}$ with $n = 4N$ and $n = 2N+1$; it is thus a generalization of the tetragonal disphenoid or tetragonal tetrahedron ($\overline{4}$) and the rhombohedron ($\overline{3}$).

[18] The term 'Miller indices' is used here also for the noncrystallographic point groups. Note that these indices do not have to be integers or rational numbers, as for the crystallographic point groups. Irrational indices, however, can always be closely approximated by integers, quite often even by small integers.

[19] A one-step procedure applies to the icosahedral 'Wyckoff position' 12*a*, the face poles and points of which are located on the fivefold axes. Here, step (ii) is redundant and can be omitted. The forms $\{01\tau\}$ and $0, y, \tau y$ are contained in the cubic point groups 23 and $m\overline{3}$ and in the cubic space groups $P23$ and $Pm\overline{3}$ as limiting cases of Wyckoff positions$\{0kl\}$ and $0, y, z$ with specialized (irrational) values of the indices and coordinates. In geometric terms, the regular pentagon-dodecahedron is a noncrystallographic 'limiting polyhedron' of the 'crystallographic' pentagon-dodecahedron and the regular icosahedron is a 'limiting polyhedron' of the 'irregular' icosahedron (*cf.* Section 3.2.1.2.2, *Crystal and point forms*).

Table 3.2.1.6
Classes of general point groups in three dimensions (N = integer ≥ 0)

Short general Hermann–Mauguin symbol, followed by full symbol where different	Schoenflies symbol	Order of group	General face form	General point form	Crystallographic groups
$4N$-gonal system (single n-fold symmetry axis with $n = 4N$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	4
$\overline{n}$	S_n	n	$\frac{1}{2}n$-gonal streptohedron	$\frac{1}{2}n$-gonal antiprism	$\overline{4}$
n/m	C_{nh}	$2n$	n-gonal dipyramid	n-gonal prism	$4/m$
$n22$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	422
nmm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$4mm$
$\overline{n}2m$	$D_{\frac{1}{2}nd}$	$2n$	n-gonal scalenohedron	$\frac{1}{2}n$-gonal antiprism sliced off by pinacoid	$\overline{4}2m$
n/mmm, $\frac{n}{m}\frac{2}{m}\frac{2}{m}$	D_{nh}	$4n$	Di-n-gonal dipyramid	Edge-truncated n-gonal prism	$4/mmm$
$(2N + 1)$-gonal system (single n-fold symmetry axis with $n = 2N + 1$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	1, 3
$\overline{n} = n \times \overline{1}$	C_{ni}	$2n$	n-gonal streptohedron	n-gonal antiprism	$\overline{1}$, $\overline{3} = 3 \times \overline{1}$
$n2$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	32
nm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$3m$
$\overline{n}m$, $\overline{n}\frac{2}{m}$	D_{nd}	$4n$	Di-n-gonal scalenohedron	n-gonal antiprism sliced off by pinacoid	$\overline{3}m$
$(4N + 2)$-gonal system (single n-fold symmetry axis with $n = 4N + 2$)					
n	C_n	n	n-gonal pyramid	Regular n-gon	2, 6
$\overline{n} = \frac{1}{2}n/m$	$C_{\frac{1}{2}nh}$	n	$\frac{1}{2}n$-gonal dipyramid	$\frac{1}{2}n$-gonal prism	$\overline{2} \equiv m$, $\overline{6} \equiv 3/m$
n/m	C_{nh}	$2n$	n-gonal dipyramid	n-gonal prism	$2/m$, $6/m$
$n22$	D_n	$2n$	n-gonal trapezohedron	Twisted n-gonal antiprism	222, 622
nmm	C_{nv}	$2n$	Di-n-gonal pyramid	Truncated n-gon	$mm2$, $6mm$
$\overline{n}2m = \frac{1}{2}n/m2m$	$D_{\frac{1}{2}nh}$	$2n$	Di-$\frac{1}{2}n$-gonal dipyramid	Truncated $\frac{1}{2}n$-gonal prism	$\overline{6}2m$
n/mmm, $\frac{n}{m}\frac{2}{m}\frac{2}{m}$	D_{nh}	$4n$	Di-n-gonal dipyramid	Edge-truncated n-gonal prism	mmm, $6/mmm$
Cubic system (for details see Table 3.2.3.2)					
23	T	12	Pentagon-tritetrahedron	Snub tetrahedron	23
$m\overline{3}$, $\frac{2}{m}\overline{3}$	T_h	24	Didodecahedron	Cube & octahedron & pentagon-dodecahedron	$m\overline{3}$
432	O	24	Pentagon-trioctahedron	Snub cube	432
$\overline{4}3m$	T_d	24	Hexatetrahedron	Cube truncated by two tetrahedra	$\overline{4}3m$
$m\overline{3}m$, $\frac{4}{m}\overline{3}\frac{2}{m}$	O_h	48	Hexaoctahedron	Cube truncated by octahedron and by rhomb-dodecahedron	$m\overline{3}m$
Icosahedral system† (for details see Table 3.2.3.3)					
235	I	60	Pentagon-hexecontahedron	Snub pentagon-dodecahedron	–
$m\overline{3}\overline{5}$, $\frac{2}{m}\overline{3}\overline{5}$	I_h	120	Hecatonicosahedron	Pentagon-dodecahedron truncated by icosahedron and by rhomb-triacontahedron	–
Cylindrical system‡					
∞	C_∞	∞	Rotating cone	Rotating circle	–
$\infty/m \equiv \overline{\infty}$	$C_{\infty h} \equiv S_\infty \equiv C_{\infty i}$	∞	Rotating double cone	Rotating finite cylinder	–
$\infty 2$	D_∞	∞	'Anti-rotating' double cone	'Anti-rotating' finite cylinder	–
∞m	$C_{\infty v}$	∞	Stationary cone	Stationary circle	–
$\infty/mm \equiv \overline{\infty}m$, $\frac{\infty}{m}\frac{2}{m} \equiv \overline{\infty}\frac{2}{m}$	$D_{\infty h} \equiv D_{\infty d}$	∞	Stationary double cone	Stationary finite cylinder	–
Spherical system§					
2∞, $\infty\infty$	K	∞	Rotating sphere	Rotating sphere	–
$m\overline{\infty}$, $\frac{2}{m}\overline{\infty}$, $\infty\infty m$	K_h	∞	Stationary sphere	Stationary sphere	–

† The Hermann–Mauguin symbols of the two icosahedral point groups are often written as 532 and $\overline{5}\overline{3}m$ (see text). ‡ Rotating and 'anti-rotating' forms in the cylindrical system have no 'vertical' mirror planes, whereas stationary forms have infinitely many vertical mirror planes. In classes ∞ and $\infty 2$, enantiomorphism occurs, *i.e.* forms with opposite senses of rotation. Class $\infty/m \equiv \overline{\infty}$ exhibits no enantiomorphism due to the centre of symmetry, even though the double cone is rotating in one direction. This can be understood as follows: The handedness of a rotating cone depends on the sense of rotation with respect to the axial direction from the base to the tip of the cone. Thus, the rotating double cone consists of two cones with opposite handedness and opposite orientations related by the (single) horizontal mirror plane. In contrast, the 'anti-rotating' double cone in class $\infty 2$ consists of two cones of equal handedness and opposite orientations, which are related by the (infinitely many) twofold axes. The term 'anti-rotating' means that upper and lower halves of the forms rotate in opposite directions. § The spheres in class 2∞ of the spherical system must rotate around an axis with at least two different orientations, in order to suppress all mirror planes. This class exhibits enantiomorphism, *i.e.* it contains spheres with either right-handed or left-handed senses of rotation around the axes (*cf.* Section 3.2.2.4, *Optical properties*). The stationary spheres in class $m\overline{\infty}$ contain infinitely many mirror planes through the centres of the spheres. Group 2∞ is sometimes symbolized by $\infty\infty$; group $m\overline{\infty}$ by $\overline{\infty}\,\overline{\infty}$ or $\infty\infty m$. The symbols used here indicate the minimal symmetry necessary to generate the groups; they show, furthermore, the relation to the cubic groups. The Schoenflies symbol K is derived from the German name *Kugelgruppe*.

(i) For the face forms the cubic point groups 23 and $m\bar{3}$ (Table 3.2.3.2), and for the point forms the cubic space groups $P23$ (195) and $Pm\bar{3}$ (200) have to be considered. For each 'initial' triplet (hkl), the set of Miller indices of the (general or special) crystal form with the same face symmetry in 23 (for group 235) or $m\bar{3}$ (for $m\bar{3}\bar{5}$) is taken. For each 'initial' triplet x, y, z, the coordinate triplets of the (general or special) position with the same site symmetry in $P23$ or $Pm\bar{3}$ are taken.

(ii) To obtain the complete set of icosahedral Miller indices and point coordinates, the 'cubic' (hkl) triplets (as rows) and x, y, z triplets (as columns) have to be multiplied with the identity matrix and with
   (a) the matrices $\boldsymbol{Y}$, $\boldsymbol{Y}^2$, $\boldsymbol{Y}^3$ and $\boldsymbol{Y}^4$ for the Miller indices;
   (b) the matrices $\boldsymbol{Y}^{-1}$, $\boldsymbol{Y}^{-2}$, $\boldsymbol{Y}^{-3}$ and $\boldsymbol{Y}^{-4}$ for the point coordinates.

This sequence of matrices ensures the same correspondence between the Miller indices and the point coordinates as for the crystallographic point groups in Table 3.2.3.2.

The matrices[20] are

$$\boldsymbol{Y} = \boldsymbol{Y}^{-4} = \begin{pmatrix} \frac{1}{2} & g & G \\ g & G & -\frac{1}{2} \\ -G & \frac{1}{2} & g \end{pmatrix}, \quad \boldsymbol{Y}^2 = \boldsymbol{Y}^{-3} = \begin{pmatrix} -g & G & \frac{1}{2} \\ G & \frac{1}{2} & -g \\ -\frac{1}{2} & g & -G \end{pmatrix},$$

$$\boldsymbol{Y}^3 = \boldsymbol{Y}^{-2} = \begin{pmatrix} -g & G & -\frac{1}{2} \\ G & \frac{1}{2} & g \\ \frac{1}{2} & -g & -G \end{pmatrix}, \quad \boldsymbol{Y}^4 = \boldsymbol{Y}^{-1} = \begin{pmatrix} \frac{1}{2} & g & -G \\ g & G & \frac{1}{2} \\ G & -\frac{1}{2} & g \end{pmatrix},$$

with[21]

$$G = \frac{\sqrt{5}+1}{4} = \frac{\tau}{2} = \cos 36^\circ = 0.80902 \simeq \frac{72}{89}$$

$$g = \frac{\sqrt{5}-1}{4} = \frac{\tau-1}{2} = \cos 72^\circ = 0.30902 \simeq \frac{17}{55}.$$

These matrices correspond to counter-clockwise rotations of 72, 144, 216 and 288° around a fivefold axis parallel to $[1\,\tau\,0]$.

The resulting indices h, k, l and coordinates x, y, z are irrational but can be approximated closely by rational (or integral) numbers. This explains the occurrence of almost regular icosahedra or pentagon-dodecahedra as crystal forms (for instance pyrite) or atomic groups (for instance B_{12} icosahedron).

Further descriptions (including diagrams) of noncrystallographic groups are contained in papers by Nowacki (1933) and A. Niggli (1963) and in the textbooks by P. Niggli (1941, pp. 78–80, 96), Shubnikov & Koptsik (1974) and Vainshtein (1994). For the geometry of polyhedra, the well known books by H. S. M. Coxeter (especially Coxeter, 1973) are recommended.

3.2.1.4.3. Sub- and supergroups of the general point groups

In Figs. 3.2.1.4 to 3.2.1.6, the subgroup and supergroup relations between the two-dimensional and three-dimensional general point groups are illustrated. It should be remembered that the index of a group–subgroup relation between two groups of order infinity may be finite or infinite. For the two spherical groups, for instance, the index is [2]; the cylindrical groups, on the other hand, are subgroups of index $[\infty]$ of the spherical groups.

Fig. 3.2.1.4 for *two dimensions* shows that the two circular groups ∞m and ∞ have subgroups of types *nmm* and *n*,

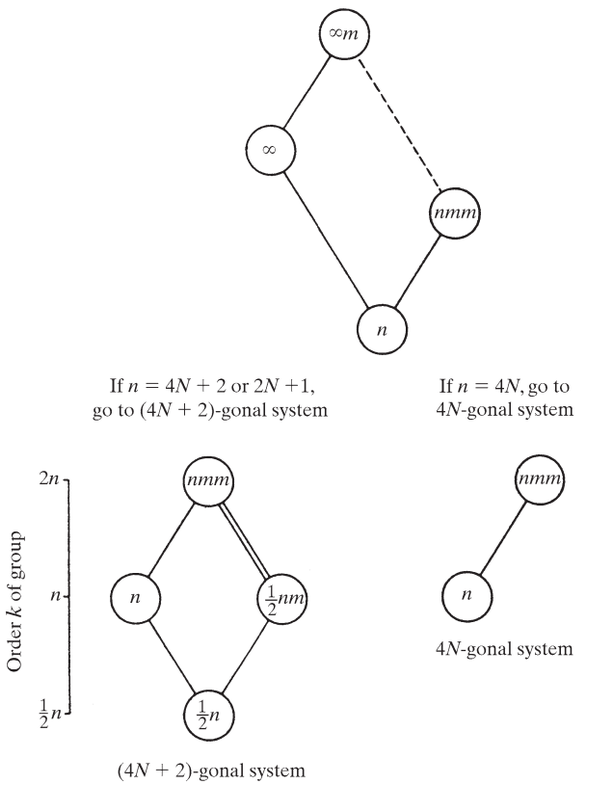


Figure 3.2.1.4
Subgroups and supergroups of the two-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, the orders are given on the left. Note that the subgroups of the two circular groups are not maximal and the diagram applies only to a specified value of N (see text). For complete examples see Fig. 3.2.1.5.

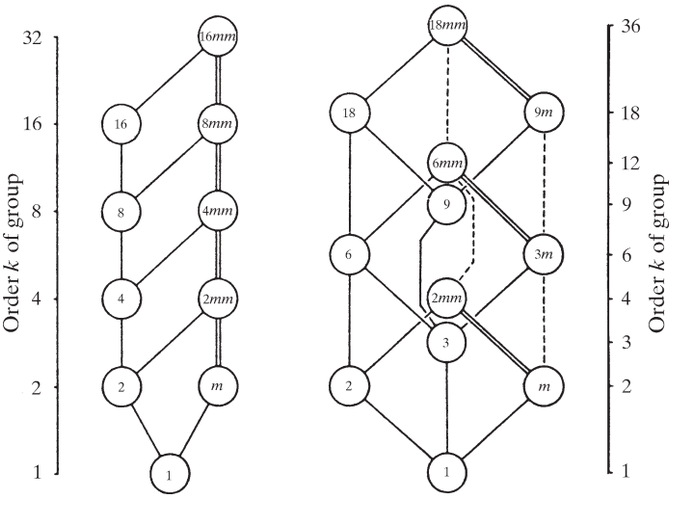


Figure 3.2.1.5
The subgroups of the two-dimensional general point groups 16*mm* (4*N*-gonal system) and 18*mm* [$(4N + 2)$-gonal system, including the $(2N + 1)$-gonal groups]. Compare with Fig. 3.2.1.4 which applies only to one value of N.

Fig. 3.2.1.4 for *two dimensions* shows that the two circular groups ∞m and ∞ have subgroups of types *nmm* and *n*,

[20] Note that for orthogonal matrices $\boldsymbol{Y}^{-1} = \boldsymbol{Y}^t$ (t = transposed).

[21] The number $\tau = 2G = 2g + 1 = (\sqrt{5}+1)/2 = 1.618034$ (Fibonacci number) is the characteristic value of the *golden section* $(\tau + 1):\tau = \tau:1$, *i.e.* $\tau(\tau - 1) = 1$. Furthermore, τ is the distance between alternating vertices of a regular pentagon of unit edge length and the distance from centre to vertex of a regular decagon of unit edge length.

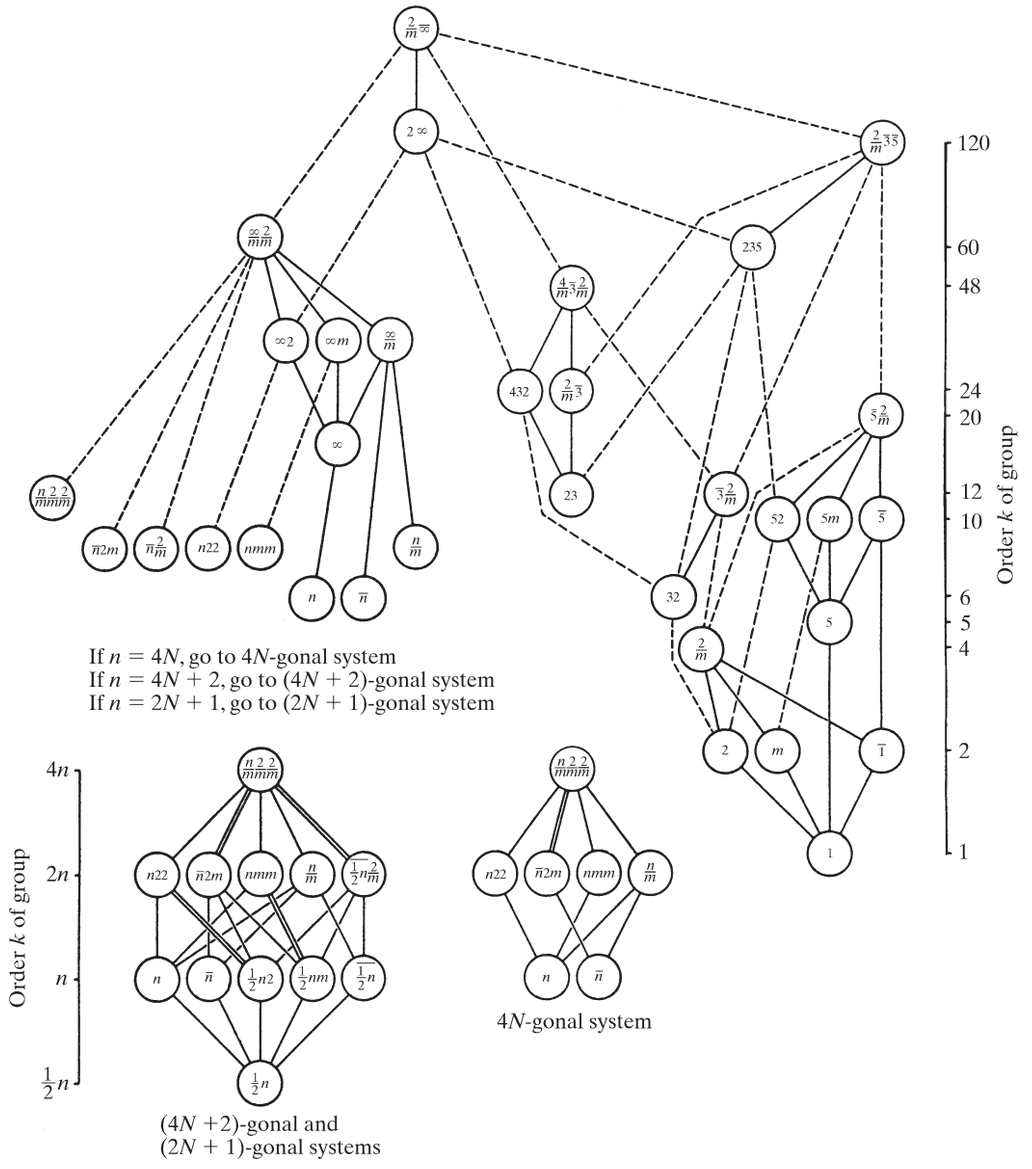


Figure 3.2.1.6
Subgroups and supergroups of the three-dimensional general point groups. Solid lines indicate maximal normal subgroups, double solid lines mean that there are two maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. For the finite groups, the orders are given on the left and on the right. Note that the subgroups of the five cylindrical groups are not maximal and that the diagram applies only to a specified value of N (see text). Only those crystallographic point groups are included that are maximal subgroups of noncrystallographic point groups, *cf.* Fig. 3.2.1.3. Full Hermann–Mauguin symbols are used.

respectively, each of index $[\infty]$. The order of the rotation point may be $n = 4N$, $n = 4N + 2$ or $n = 2N + 1$. In the first case, the subgroups belong to the $4N$-gonal system, in the latter two cases, they belong to the $(4N + 2)$-gonal system. [In the diagram of the $(4N + 2)$-gonal system, the $(2N + 1)$-gonal groups appear with the symbols $\frac{1}{2}nm$ and $\frac{1}{2}n$.] The subgroups of the circular groups are not maximal because for any given value of N there exists a group with $N' = 2N$ which is both a subgroup of the circular group and a supergroup of the initial group.

The subgroup relations, for a specified value of N, within the $4N$-gonal and the $(4N + 2)$-gonal system, are shown in the lower part of the figure. They correspond to those of the crystallographic groups. A finite number of further maximal subgroups is obtained for lower values of N, until the crystallographic groups (Fig. 3.2.1.2) are reached. This is illustrated for both systems in Fig. 3.2.1.5.

Fig. 3.2.1.6 for *three dimensions* illustrates that the two spherical groups $2/m\overline{\infty}$ and 2∞ each have one infinite set of cylindrical maximal conjugate subgroups, as well as one infinite set of cubic and one infinite set of icosahedral maximal finite conjugate subgroups, all of index $[\infty]$.

Each of the two icosahedral groups 235 and $2/m\,\bar{3}\,\bar{5}$ has one set of five cubic, one set of six pentagonal and one set of ten trigonal maximal conjugate subgroups of indices [5], [6] and [10], respectively (*cf.* Section 3.2.1.4.2, *The two icosahedral groups*); they are listed on the right of Fig. 3.2.1.6. For the crystallographic groups, Fig. 3.2.1.3 applies. The subgroup types of the five cylindrical point groups are shown on the upper left part of Fig. 3.2.1.6. As explained above for two dimensions, these subgroups are *not maximal* and of index $[\infty]$. Depending upon whether the main symmetry axis has the multiplicity $4N$, $4N + 2$ or $2N + 1$, the subgroups belong to the $4N$-gonal, $(4N + 2)$-gonal or $(2N + 1)$-gonal system.

The subgroup and supergroup relations within these three systems are displayed in the lower left part of Fig. 3.2.1.6. They are analogous to the crystallographic groups. To facilitate the

use of the diagrams, the $(4N+2)$-gonal and the $(2N+1)$-gonal systems are combined, with the consequence that the five classes of the $(2N+1)$-gonal system now appear with the symbols $\overline{\frac{1}{2}n}\frac{2}{m}$, $\frac{1}{2}n2$, $\frac{1}{2}nm$, $\overline{\frac{1}{2}n}$ and $\frac{1}{2}n$. Again, the diagrams apply to a specified value of N. A finite number of further maximal subgroups is obtained for lower values of N, until the crystallographic groups (Fig. 3.2.1.3) are reached (*cf.* the two-dimensional examples in Fig. 3.2.1.5).

3.2.2. Point-group symmetry and physical properties of crystals

By H. Klapper and Th. Hahn

In the previous section (Section 3.2.1), the crystallographic and noncrystallographic point groups are treated under geometrical aspects only. In the present section the point-group symmetries of the physical properties are considered. Among the physical properties, those represented by tensors are accessible to a mathematical treatment of their symmetries, which are apparent by the invariance of tensor components under symmetry operations. For more details the reader is referred to Nye (1957, 1985), Paufler (1986), Schwarzenbach & Chapuis (2006) and Shuvalov (1988). A similar comprehensive treatment of non-tensorial properties, such as cleavage, plasticity, hardness or crystal growth does not exist, but these properties are, of course, also governed by the crystallographic point-group symmetry.

3.2.2.1. General restrictions on physical properties imposed by symmetry

3.2.2.1.1. Neumann's principle

Neumann's principle (Neumann, 1885) describes the relation between the symmetry $\mathcal{Q}$ of a physical property and the crystallographic point group $\mathcal{P}$ of a crystal. It states that the symmetry of any physical property of a crystal is higher than, or at least equal to, its crystallographic point-group symmetry, or in the language of groups, the symmetry $\mathcal{Q}$ of any physical property of a crystal is a proper or improper supergroup of its crystallographic symmetry $\mathcal{P}$: $\mathcal{Q} \subseteq \mathcal{P}$. This is easily illustrated for polar second-rank tensors, which are represented by ellipsoids and hyperboloids. The representation surfaces of triclinic, monoclinic and orthorhombic crystals are general ellipsoids or hyperboloids of symmetry $\mathcal{Q} = 2/m\,2/m\,2/m$, which is a proper supergroup of all triclinic, monoclinic and orthorhombic point groups with the only exception of the orthorhombic holohedry $\mathcal{P} = 2/m\,2/m\,2/m$, for which the two symmetries are the same. For the uniaxial crystals of the trigonal, tetragonal and hexagonal systems the representation ellipsoids and hyperboloids have rotation symmetries with the cylindrical point group $\mathcal{Q} = \infty/m\,2/m$ (see Table 3.2.1.6), which is a proper supergroup of all uniaxial crystallographic point groups. For cubic crystals, second-rank tensors are isotropic and represented by a sphere with point-group symmetry $\mathcal{Q} = 2/m\,\overline{\infty}$ $(\infty\infty m)$, a proper supergroup of all cubic crystallographic point groups. For more details the reader is referred to Paufler (1986) and Authier (2014). A short resume is given by Klapper & Hahn (2005).

As a consequence of the invariance of tensor components under a symmetry operation (or alternatively: under a transformation of the coordinate system to a symmetry-equivalent one), some of the tensor components are equal or even zero. The number of independent components decreases when the symmetry of the crystal increases. Thus, an increase of the point-group symmetry from 1 (triclinic) to $4/m\,\bar{3}\,2/m$ (cubic) or to the sphere group $\infty\infty m$ (*i.e.* isotropy) reduces the number of tensor components for symmetrical second-rank tensors from 6 to 1. Even more drastic is this reduction for all tensors of odd rank (such as pyroelectricity and piezoelectricity) or axial tensors of second rank (*e.g.* optical activity): all components are zero if an inversion centre is present, *i.e.* properties described by these tensors do not exist in centrosymmetric crystals (see the textbooks of tensor physics mentioned above). These properties, which exist only in noncentrosymmetric crystals are, as a rule, the most important ones, not only for physical applications but also for structure determination, because they allow a proof of the absence of a symmetry centre.

For the description of noncentrosymmetric crystals and their specific properties, certain notions are of importance and these are explained in the following two sections.

3.2.2.1.2. Curie's principle

Curie's principle (Curie, 1894) describes the crystallographic symmetry $\mathcal{P}_F$ of a macroscopic crystal which is subject to an external influence F, for example to an electric field $\mathbf{E}$, to uniaxial stress σ_{ii}, to a temperature change ΔT *etc*. For this treatment, the point-group symmetries $\mathcal{R}$ of the external influences (Curie groups) are defined as follows (see Authier, 2014, p. 11; Paufler, 1986, p. 29):

Homogeneous electric field $\mathbf{E}$: $\mathcal{R} = \infty m$ (polar continuous rotation axis with 'parallel' mirror planes, *i.e.* symmetry of a stationary cone) [Note that a rotating cone (left- or right-handed) represents geometrically the polar enantiomorphous group ∞; a stationary cone represents the polar group ∞m with 'vertical' mirror planes, *cf.* Section 3.2.1.4.1.];

Homogeneous magnetic field $\mathbf{H}$: $\mathcal{R} = \infty/m$ (symmetry of a rotating cylinder);

Uniaxial stress σ_{ii}: $\mathcal{R} = \infty/m\,2/m$ (symmetry of a stationary centrosymmetric cylinder);

Temperature change ΔT or hydrostatic pressure p (scalars): $\mathcal{R} = 2/m\,\overline{\infty}$ $(\infty\infty m)$ (symmetry of a stationary centrosymmetric sphere);

Shear stress σ_{ij}: $\mathcal{R} = 2/m\,2/m\,2/m$ (orthorhombic).

According to Curie's principle, the point-group symmetry $\mathcal{P}_F$ of the crystal under the external field F is the intersection symmetry of the two point groups: $\mathcal{P}$ of the crystal without field and $\mathcal{R}$ of the field without crystal: $\mathcal{P}_F = \mathcal{R} \cap \mathcal{P}$; *i.e.* $\mathcal{P}_F$ is a (proper or improper) subgroup of both groups $\mathcal{R}$ and $\mathcal{P}$.

As examples we consider the effect of an electric field ($\mathcal{R} = \infty m$) and of a uniaxial stress ($\mathcal{R} = \infty/m\,2/m$) along one of the (four) threefold rotoinversion axes $\bar{3}$ of cubic crystals with point groups $\mathcal{P} = 2/m\,\bar{3}$ and $\mathcal{P} = 4/m\,\bar{3}\,2/m$.

Electric field parallel to [111]:

$2/m\,\bar{3} \cap \infty m$:	$\mathcal{P}_F = 3$	along [111] (polar, pyroelectric, optically active; *cf*. Sections 3.2.2.5 and 3.2.2.4.2)
$4/m\,\bar{3}\,2/m \cap \infty m$:	$\mathcal{P}_F = 3m$	along [111] (polar, pyroelectric, not optically active)

Table 3.2.2.1
The 11 Laue classes, the 21 noncentrosymmetric crystallographic point groups (crystal classes) and the occurrence (+) of specific crystal properties

The number of non-zero independent tensor components is given in parentheses. For comparison, the icosahedral and the sphere groups (isotropy) are added. For first-rank tensors the direction [*uvw*] of the property vector is given. There are 10 pyroelectric, 20 piezoelectric, 11 enantiomorphic and 15 optically active crystal classes.

Crystal system	Laue class	Noncentrosymmetric point group	First-rank tensor (*e.g.* pyroelectricity, piezoelectricity under hydrostatic pressure)	Third-rank tensor (*e.g.* piezoelectricity, second-harmonic generation)	Enantiomorphism	Axial second-rank tensor (optical activity = optical gyration)
Triclinic	$\bar{1}$	1	+ (3) [*uvw*]	+ (18)	+	+ (6)
Monoclinic	$2/m$	2	+ (1) [010]†	+ (8)	+	+ (4)
		m	+ (2) [*u*0*w*]†	+ (10)	−	+ (2)
Orthorhombic	$2/m\,2/m\,2/m$	222	−	+ (3)	+	+ (3)
		$mm2$	+ (1) [001]	+ (5)	−	+ (1)
Tetragonal	$4/m$	4	+ (1) [001]	+ (4)	+	+ (2)
		$\bar{4}$	−	+ (4)	−	+ (2)
	$4/m\,2/m\,2/m$	422	−	+ (1)	+	+ (2)
		$4mm$	+ (1) [001]	+ (3)	−	−
		$\bar{4}2m$	−	+ (2)	−	+ (1)
Trigonal	$\bar{3}$	3	+ (1) [001]‡	+ (6)	+	+ (2)
	$\bar{3}\,2/m$	32	−	+ (2)	+	+ (2)
		$3m$	+ (1) [001]‡	+ (4)	−	−
Hexagonal	$6/m$	6	+ (1) [001]	+ (4)	+	+ (2)
		$\bar{6}$	−	+ (2)	−	−
	$6/m\,2/m\,2/m$	622	−	+ (1)	+	+ (2)
		$6mm$	+ (1) [001]	+ (3)	−	−
		$\bar{6}2m$	−	+ (1)	−	−
Cubic	$2/m\,\bar{3}$	23	−	+ (1)	+	+ (1)
	$4/m\,\bar{3}\,2/m$	432	−	−	+	+ (1)
		$\bar{4}3m$	−	+ (1)	−	−
Icosahedral	$m\bar{3}\bar{5}$ ($\bar{5}\bar{3}m$)	235 (532)	−	−	+	+ (1)
Spherical	$m\overline{\infty}$ ($\infty\infty m$)	2∞ ($\infty\infty$)	−	−	+	+ (1)

† Unique axis *b*. ‡ Hexagonal axes.

Uniaxial stress parallel to [111]:

$2/m\,\bar{3} \cap \infty/m\,2/m$: $\mathcal{P}_F = \bar{3}$ along [111]
$4/m\,\bar{3}\,2/m \cap \infty/m\,2/m$: $\mathcal{P}_F = \bar{3}\,2/m$ along [111].

Note that, in contrast to uniaxial stress, the electric field destroys centrosymmetry, leading to pyroelectricity and even optical gyration. The polarity and the gyration sense are reversed upon reversal of the electric field. If the electric field and the uniaxial stress were applied to an arbitrary (non-symmetry) direction of the above cubic crystals, point groups 1 and $\bar{1}$ would result in the two cases.

If a scalar influence $\mathcal{R} = 2/m\,\overline{\infty}$ ($\infty\infty m$) (centrosymmetric sphere group) is applied to a crystal, its symmetry $\mathcal{P}_F = \mathcal{P}$ is not changed, provided that no phase transition is induced.

For further reading on tensor properties of crystals the textbooks in the references and *International Tables for Crystallography*, Volume D (2014) are recommended.

3.2.2.1.3. Enantiomorphism, enantiomerism, chirality, dissymmetry

All these terms refer to the same symmetry restriction, the absence of improper rotations (rotoinversions, rotoreflections) in a crystal or in a molecule. This implies in particular the absence of a centre of symmetry, $\bar{1}$, and of a mirror plane, $m = \bar{2}$, but also of a $\bar{4}$ axis. As a consequence, such *chiral* crystals or molecules can occur in two different forms, which are related as a right and a left hand; hence, they are called right-handed and left-handed forms. These two forms of a molecule or a crystal are mirror-related and not superimposable (not congruent). Thus, the only symmetry operations that are allowed for *chiral* objects are proper rotations. Such objects are also called *dissymmetric*, in contrast to *asymmetric* objects, which have no symmetry.

The terms *enantiomerism* and *chirality* are mainly used in chemistry and applied to molecules, whereas the term *enantiomorphism* is preferred in crystallography if reference is made to crystals.

Enantiomorphic crystals, as well as solutions or melts containing chiral molecules of one handedness, exhibit optical activity (*cf.* Section 3.2.2.4.2). Crystals and molecules of the other handedness show optical activity with the opposite sense of rotation. For this reason, two molecules of opposite chirality are also called *optical isomers*.

Chiral molecules form enantiomorphic crystals of the corresponding handedness. These crystals belong, therefore, to one of the 11 crystal classes allowing enantiomorphism (Table 3.2.2.1). Racemic mixtures (containing equal amounts of molecules of each chirality), however, may crystallize in non-enantiomorphic or even centrosymmetric crystal classes. Racemization (*i.e.* the switching of molecules from one chirality to the other) of an optically active melt or solution can occur in some cases during crystallization, leading to non-enantiomorphic crystals.

Table 3.2.2.2
Polar axes and nonpolar directions in the 21 noncentrosymmetric crystal classes

All directions normal to an evenfold rotation axis and along rotoinversion axes are nonpolar. All directions other than those in the column 'Nonpolar directions' are polar. A symbol like [$u0w$] refers to the set of directions obtained for all possible values of u and w, in this case to all directions normal to the b axis, *i.e.* parallel to the plane (010). Symmetry-equivalent sets of nonpolar directions are placed between semicolons; the sequence of these sets follows the sequence of the symmetry directions in Table 2.1.3.1.

System	Class	Polar (symmetry) axes	Nonpolar directions
Triclinic	1	None†	None
Monoclinic Unique axis b	2	[010]	[$u0w$]
	m	None†	[010]
Monoclinic Unique axis c	2	[001]	[$uv0$]
	m	None†	[001]
Orthorhombic	222	None	[$0vw$]; [$u0w$]; [$uv0$]
	$mm2$	[001]	[$uv0$]
Tetragonal	4	[001]	[$uv0$]
	$\bar{4}$	None	[001]; [$uv0$]
	422	None	[$uv0$]; [$0vw$] [$u0w$]; [uuw] [$u\bar{u}w$]
	$4mm$	[001]	[$uv0$]
	$\bar{4}2m$	None	[$uv0$]; [$0vw$] [$u0w$]
	$\bar{4}m2$	None	[$uv0$]; [uuw] [$u\bar{u}w$]
Trigonal (Hexagonal axes)	3	[001]	None
	321	[100], [010], [$\bar{1}\bar{1}0$]	[$u2uw$] [$\bar{2}u\bar{u}w$] [$u\bar{u}w$]
	312	[$1\bar{1}0$], [120], [$\bar{2}\bar{1}0$]	[uuw] [$\bar{u}0w$] [$0\bar{v}w$]
	$3m1$	[001]	[100] [010] [$\bar{1}\bar{1}0$]
	$31m$	[001]	[$1\bar{1}0$] [120] [$\bar{2}\bar{1}0$]
Trigonal (Rhombohedral axes)	3	[111]	None
	32	[$1\bar{1}0$], [$01\bar{1}$], [$\bar{1}01$]	[uuw] [uvv] [uvu]
	$3m$	[111]	[$1\bar{1}0$] [$01\bar{1}$] [$\bar{1}01$]
Hexagonal	6	[001]	[$uv0$]
	$\bar{6}$	None	[001]
	622	None	[$u2uw$] [$\bar{2}u\bar{u}w$] [$u\bar{u}w$] [uuw] [$\bar{u}0w$] [$0\bar{v}w$]
	$6mm$	[001]	[$uv0$]
	$\bar{6}m2$	[$1\bar{1}0$], [120], [$\bar{2}\bar{1}0$]	[uuw] [$\bar{u}0w$] [$0\bar{v}w$]
	$\bar{6}2m$	[100], [010], [$\bar{1}\bar{1}0$]	[$u2uw$] [$\bar{2}u\bar{u}w$] [$u\bar{u}w$]
Cubic	23	Four threefold axes along ⟨111⟩	[$0vw$] [$u0w$] [$uv0$]
	$\bar{4}3m$		[$0vw$] [$u0w$] [$uv0$]
	432	None	[$0vw$] [$u0w$] [$uv0$]; [uuw] [uvv] [uvu]; [$u\bar{u}w$] [$uv\bar{v}$] [$\bar{u}vu$]

† In class 1 any direction is polar; in class m all directions except [010] (or [001]) are polar.

Enantiomorphic crystals can also be built up from achiral molecules or atom groups. In these cases, the achiral molecules or atom groups form chiral configurations in the structure. The best known examples are quartz and $NaClO_3$. For details, reference should be made to Rogers (1975).

3.2.2.1.4. Polar directions, polar axes, polar point groups

A *direction* is called *polar* if its two directional senses are geometrically or physically different. A *polar symmetry direction* of a crystal is called a *polar axis.* Only proper rotation or screw axes can be polar. The polar and nonpolar directions in the 21 noncentrosymmetric point groups are listed in Table 3.2.2.2.

The terms *polar point group* or *polar crystal class* are used in two different meanings. In crystal physics, a crystal class is considered as polar if it allows the existence of a permanent dipole moment, *i.e.* if it is capable of pyroelectricity (*cf.* Section 3.2.2.5). In crystallography, however, the term *polar crystal class* is frequently used synonymously with *noncentrosymmetric crystal class.* The synonymous use of polar and acentric, however, can be misleading, as is shown by the following example. Consider an optically active liquid. Its symmetry can be represented as a right-handed or a left-handed sphere (*cf.* Sections 3.2.1.4 and 3.2.2.4). The optical activity is isotropic, *i.e.* magnitude and rotation sense are the same in any direction and its counterdirection. Thus, no polar direction exists, although the liquid is noncentrosymmetric with respect to optical activity.

According to Neumann's principle, information about the point group of a crystal may be obtained by the observation of physical effects. Here, the term 'physical properties' includes crystal morphology and etch figures. The use of any of the techniques described below does not necessarily result in the complete determination of symmetry but, when used in conjunction with other methods, much information may be obtained. It is important to realize that the evidence from these methods is often negative, *i.e.* that symmetry conclusions drawn from such evidence must be considered as only provisional.

In the following sections, the physical properties suitable for the determination of symmetry are outlined briefly. For more details, reference should be made to the monographs by Bhagavantam (1966), Nye (1957) and Wooster (1973).

3.2.2.2. Morphology

If a crystal shows well developed faces, information on its symmetry may be derived from the external form of the crystal. By means of the optical goniometer, faces related by symmetry can be determined even for crystals far below 1 mm in diameter. By this procedure, however, only the eigensymmetry (*cf.* Section 3.2.1.2.2) of the crystal morphology (which may consist of a single form or a combination of forms) can be established. The determination of the point group is unique in all cases where the observed eigensymmetry group is compatible with only one generating group.

Column 6 in Table 3.2.1.3 lists all point groups for which a given crystal form (characterized by its name and eigensymmetry) can occur. In 19 cases, the point group can be uniquely determined because only one entry appears in column 6. These crystal forms are always characteristic general forms, for which eigensymmetry and generating point-group symmetry are identical. They belong to the 19 point groups with more than one symmetry direction.

If a crystal exhibits a combination of forms which by themselves do not permit unambiguous determination of the point group, those generating point groups are possible that are common to all crystal forms of the combination. The mutual orientation of the forms, if variable, has to be taken into account, too.

Example

Two tetragonal pyramids, each of eigensymmetry $4mm$, rotated with respect to each other by an angle $\neq 45°$, determine the point group 4 uniquely because the eigensymmetry of the *combination* is only 4.

In practice, however, unequal or incomplete development of the faces of a form often simulates a symmetry that is lower than the actual crystal symmetry. In such cases, or when the

morphological analysis is ambiguous, the crystallization of a small amount of the compound on a seed crystal, ground to a sphere, is useful. By this procedure, faces of additional forms (and often of the characteristic general form) appear as small facets on the sphere and their interfacial angles can be measured.

In favourable cases, even the space group can be derived from the morphology of a crystal: this is based on the so-called *Bravais–Donnay–Harker principle*. A textbook description is given by Phillips (1971, ch. 13).

Furthermore, measurements of the interfacial angles by means of the optical goniometer permit the determination of the relative dimensions of a 'morphological unit cell' with good accuracy. Thus, for instance, the interaxial angles α, β, γ and the axial ratio a:b:c of a triclinic crystal may be derived. The ratio a:b:c, however, may contain an uncertainty by an integral factor with respect to the actual cell edges of the crystal. This means that any one unit length may have to be multiplied by an integer in order to obtain correspondence to the 'structural' unit cell.

3.2.2.3. Etch figures

Additional information on the point group of a crystal can be gained from the face symmetry, which is usually determined by observation of etch figures, striations and other face markings. Etch pits are produced by heating the crystal in vacuum (evaporation from the surface) or by attacking it with an appropriate reagent, which should not be optically active. The etch pits generally appear at the end points of dislocation lines on the face. They exhibit the symmetry of one of the ten two-dimensional point groups which, in general,[22] corresponds to the symmetry of the crystal face under investigation.

The observation of etch figures is important when the morphological analysis is ambiguous (*cf.* Section 3.2.2.2). For instance, a tetragonal pyramid, which is compatible with point groups 4 and 4*mm*, can be uniquely attributed to point group 4 if its face symmetry is found to be 1. For face symmetry *m*, group 4*mm* would result. The (oriented) face symmetries of the 47 crystal forms in the various point groups are listed in column 6 of Table 3.2.1.3 and in column 3 of Table 3.2.3.2.

In noncentrosymmetric crystals, the etch pits on parallel but opposite faces, even though they have the same symmetry, may be of different size or shape, thus proving the absence of a symmetry centre. Note that the orientation of etch pits with respect to the edges of the face is significant (*cf.* Buerger, 1956), as well as the mutual arrangement of etch pits on opposite faces. Thus, for a pinacoid with face symmetry 1, the possible point groups $\overline{1}$, 2 and *m* of the crystal can be distinguished by the mutual orientation of etch pits on the two faces. Moreover, twinning by merohedry and the true symmetry of the two (or more) twin partners ('twin domains') may be detected.

The method of etching can be applied not only to growth faces but also to cleavage faces or arbitrarily cut faces.

3.2.2.4. Optical properties

Optical studies provide good facilities with which to determine the symmetry of transparent crystals. The following optical properties may be used.

Table 3.2.2.3
Categories of crystal systems distinguished according to the different forms of the indicatrix

Crystal system	Shape of indicatrix	Optical character
Cubic	Sphere	Isotropic (not doubly refracting)
Tetragonal, Trigonal, Hexagonal	Rotation ellipsoid	Uniaxial } Anisotropic (doubly refracting)
Orthorhombic, Monoclinic, Triclinic	General ellipsoid	Biaxial } Anisotropic (doubly refracting)

3.2.2.4.1. Refraction

The dependence of the *refractive index* on the vibration direction of a plane-polarized light wave travelling through the crystal can be obtained from the optical indicatrix. This surface is an ellipsoid, which can degenerate into a rotation ellipsoid or even into a sphere. Thus, the lowest symmetry of the property 'refraction' is 2/*m* 2/*m* 2/*m*, the point group of the general ellipsoid. According to the three different forms of the indicatrix, three categories of crystal systems have to be distinguished (Table 3.2.2.3).

The orientation of the indicatrix is related to the symmetry directions of the crystal. In tetragonal, trigonal and hexagonal crystals, the rotation axis of the indicatrix (which is the unique optic axis) is parallel to the main symmetry axis. For orthorhombic crystals, the three principal axes of the indicatrix are oriented parallel to the three symmetry directions of the crystal. In the monoclinic system, one of the axes of the indicatrix coincides with the monoclinic symmetry direction, whereas in the triclinic case, the indicatrix can, in principle, have any orientation relative to a chosen reference system. Thus, in triclinic and, with restrictions, in monoclinic crystals, the *orientation* of the indicatrix can change with wavelength λ and temperature T (orientation dispersion). In any system, the *size* of the indicatrix and, in all but the cubic system, its *shape* can also vary with λ and T.

When studying the symmetry of a crystal by optical means, note that strain can lower the apparent symmetry owing to the high sensitivity of optical properties to strain.

3.2.2.4.2. Optical activity

The symmetry information obtained from *optical activity* is quite different from that given by optical refraction. Optical activity is in principle confined to the 21 noncentrosymmetric classes but it can occur in only 15 of them (Table 3.2.2.1). In the 11 enantiomorphism classes, a single crystal is either right- or left-handed. In the four non-enantiomorphous classes *m*, *mm*2, $\overline{4}$ and $\overline{4}2m$, optical activity may also occur; here directions of both right- and left-handed rotations of the plane of polarization exist in the same crystal. In the other six noncentrosymmetric classes, 3*m*, 4*mm*, $\overline{6}$, 6*mm*, $\overline{6}2m$, $\overline{4}3m$, optical activity is not possible.

In the two cubic enantiomorphous classes 23 and 432, the optical activity is isotropic and can be observed along any direction.[23] For the other optically active crystals, the rotation of the plane of polarization can, in practice, be detected only in directions parallel (or approximately parallel) to the optic axes. This is because of the dominating effect of double refraction. No optical activity, however, is present along an inversion axis or along a direction parallel or perpendicular to a

[22] It should be noted, however, that asymmetric etch figures may occur that are due, for example, to an inclination of dislocation lines against the surface.

[23] This property can be represented by enantiomorphic spheres of point group 2∞, *cf.* Table 3.2.1.6.

mirror plane. Thus, no activity occurs along the optic axis in crystal classes $\overline{4}$ and $\overline{4}2m$. In classes m and $mm2$, no activity can be present along the two optic axes if these axes lie in m. If they are not parallel to m, they show optical rotation(s) of opposite sense.

3.2.2.4.3. Second-harmonic generation (SHG)

Light waves passing through a noncentrosymmetric crystal induce new waves of twice the incident frequency. This second-harmonic generation is due to the nonlinear optical susceptibility. The *second-harmonic coefficients* form a third-rank tensor, which is subject to the same symmetry constraints as the piezoelectric tensor (see Section 3.2.2.6). Thus, only 20 noncentrosymmetric crystals, except those of class 432, can show the second-harmonic effect; *cf.* Table 3.2.2.1.

Second-harmonic generation is a powerful method of testing crystalline materials for the absence of a symmetry centre. With an appropriate experimental device, very small amounts (less than 10 mg) of powder are sufficient to detect the second-harmonic signals, even for crystals with small deviations from centrosymmetry (Dougherty & Kurtz, 1976).

3.2.2.5. Pyroelectricity and ferroelectricity

In principle, *pyroelectricity* can only exist in crystals with a permanent electric dipole moment. This moment is changed by heating and cooling, thus giving rise to electric charges on certain crystal faces, which can be detected by simple experimental procedures.

An electric dipole moment can be present only along a polar direction that has no symmetry-equivalent directions.[24] Such polar directions occur in the following ten classes: $6mm$, $4mm$, and their subgroups 6, 4, $3m$, 3, $mm2$, 2, m, 1 (*cf.* Table 3.2.2.1). In point groups with a rotation axis, the electric moment is along this axis. In class m, the electric moment is parallel to any direction in the mirror plane (direction $[u0w]$). In class 1, any direction $[uvw]$ is possible. In point groups 1 and m, besides a change in magnitude, a directional variation of the electric moment can also occur during heating or cooling.

In practice, it is difficult to prevent strains from developing throughout the crystal as a result of temperature gradients in the sample. This gives rise to piezoelectrically induced charges superposed on the true pyroelectric effect. Consequently, when the development of electric charges by a change in temperature is observed, the only safe deduction is that the specimen must lack a centre of symmetry. Failure to detect pyroelectricity may be due to extreme weakness of the effect, although modern methods are very sensitive.

A crystal is *ferroelectric* if the direction of the permanent electric dipole moment can be changed by an electric field. Thus, ferroelectricity can only occur in the ten pyroelectric crystal classes, mentioned above.

3.2.2.6. Piezoelectricity

In piezoelectric crystals, an electric dipole moment can be induced by compressional and torsional stress. For a uniaxial compression, the induced moment may be parallel, normal or inclined to the compression axis. These cases are called longitudinal, transverse or mixed compressional piezoeffect, respectively. Correspondingly, for torsional stress, the electric moment may be parallel, normal or inclined to the torsion axis.

The *piezoelectricity* is described by a third-rank tensor, the moduli of which vanish for all centrosymmetric point groups. Additionally, in class 432, all piezoelectric moduli are zero owing to the high symmetry. Thus, piezoelectricity can only occur in 20 noncentrosymmetric crystal classes (Table 3.2.2.1).

The piezoelectric point groups 422 and 622 show the following peculiarity: there is no direction for which a longitudinal component of the electric moment is induced under uniaxial compression. Thus, no longitudinal or mixed compressional effects occur. The moment is always normal to the compression axis (pure transverse compressional effect). This means that, with the compression pistons as electrodes, no electric charges can be found, since only transverse compressional or torsional piezoeffects occur. In all other piezoelectric classes, there exist directions in which both longitudinal and transverse components of the electric dipole moment are induced under uniaxial compression.

An electric moment can also develop under hydrostatic pressure. This kind of piezoelectricity, like pyroelectricity, can be represented by a first-rank tensor (vector), whereby the hydrostatic pressure is regarded as a scalar. Thus, piezoelectricity under hydrostatic pressure is subject to the same symmetry constraints as pyroelectricity.

Like 'second-harmonic generation' (Section 3.2.2.4.3), the piezoelectric effect is very useful for testing crystals for the absence of a symmetry centre. There exist powerful methods for testing powder samples or even small single crystals. In the old technique of Giebe & Scheibe (*cf.* Wooster & Brenton, 1970), the absorption and emission of radio-frequency energy by electromechanical oscillations of piezoelectric particles are detected. In the more modern method of observing 'polarization echoes', radio-frequency pulses are applied to powder samples. By this procedure, electromechanical vibration pulses are induced in piezoelectric particles, the echoes of which can be detected (*cf.* Melcher & Shiren, 1976).

[24] In the literature, the requirement for pyroelectricity is frequently expressed as 'a unique (or singular) polar axis'. This term, however, is misleading for point groups 1 and m.

3.2.3. Tables of the crystallographic point-group types

By H. Klapper, Th. Hahn and M. I. Aroyo

The crystallographic point-group types are listed in Tables 3.2.3.1 and 3.2.3.2 for two-dimensional and for three-dimensional space, respectively. No listings are presented for the noncrystallographic point-group types (*i.e.* having axes of orders other than 1, 2, 3, 4 and 6), but their symbols can be found in Tables 3.2.1.5, 3.2.1.6 and 3.2.3.3 (*cf.* Section 3.2.1.4 for a review of noncrystallographic point groups). The two icosahedral point groups 235 and $m\bar{3}\bar{5}$ are treated in detail in Section 3.2.1.4.2, while their crystallographic data are shown in Table 3.2.3.3.

There is a physical difference between the point groups of crystals and those of molecules. For a molecule, the point group is the set of all symmetry operations that map its atoms onto one another. Macroscopic crystals, however, hardly ever exhibit their ideal symmetry because of the defects that occur during crystal growth. For a crystal, its point group is the set of all symmetry operations that map the set of the vectors normal to the crystal faces onto one another; it does not operate in point space, but in vector space.

In Tables 3.2.3.1 and 3.2.3.2 the point-group types are presented for crystals as well as for molecules. However, parts of the tables concern either crystals only or molecules only. The names of crystal forms in the fifth column (in roman type) and the *hkl* face indices in the last column are only relevant for crystals. The names of the point forms in the second line of each pair of entries in the fifth column (given in italics) and the other data (multiplicities, Wyckoff letters, site symmetries and sets of symmetry-equivalent coordinates) concern both crystals and molecules. However, for point groups with an origin fixed by symmetry, the Wyckoff position with the Wyckoff letter *o* is only of interest for molecules.

Because the meanings of the entries are not identical for crystals and for molecules, they are not explained here, but in Sections 3.2.1 (for crystals) and 3.2.4 (for molecules).

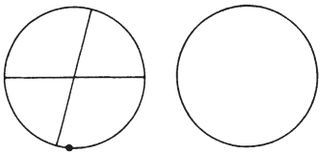
(*continued on page* 772)

Table 3.2.3.1
The ten two-dimensional crystallographic point groups

The point groups are listed in blocks according to crystal system and are specified by their Hermann–Mauguin symbols. For each point group, the stereographic projections show (on the left) the general position and (on the right) the symmetry elements.
The list of Wyckoff positions includes:
Columns 1 to 4: multiplicity, Wyckoff letter, oriented site-symmetry symbol, coordinate doublets;
Under the stereographic projections: edge forms (in roman type) and point forms (in italics); if there are two entries, the second entry refers to a limiting (noncharacteristic) form;
Last column: Miller indices of equivalent edges [for hexagonal groups, Bravais–Miller indices (*hki*) are used].

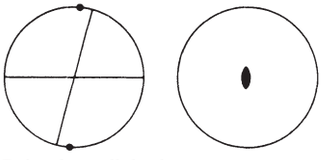
OBLIQUE SYSTEM

1



1	*a*	1	x, y	Single edge *Single point*	(hk)

2



2	*a*	1	x, y $\bar{x}, \bar{y}$	Pair of parallel edges *Line segment through origin*	(hk) $(\bar{h}\bar{k})$
1	*o*	2	0, 0	*Point in origin*	

Table 3.2.3.1 (continued)

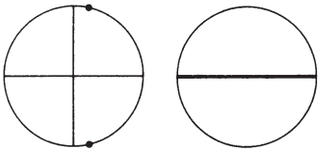
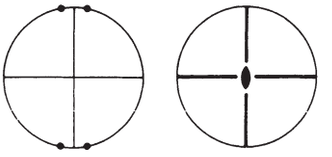
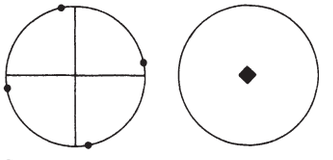
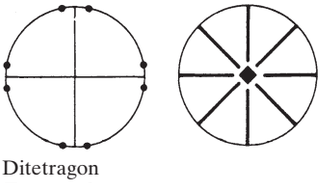
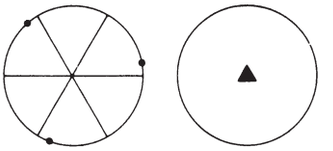
RECTANGULAR SYSTEM					
m					
2	*b*	1	x, y $\bar{x}, y$	Pair of edges *Line segment*	(hk) $(\bar{h}k)$
				Pair of parallel edges *Line segment through origin*	(10) $(\bar{1}0)$
1	*a*	*.m.*	$0, y$	Single edge *Single point*	(01) or $(0\bar{1})$
2*mm*					
4	*c*	1	x, y $\bar{x}, \bar{y}$ $\bar{x}, y$ $x, \bar{y}$	Rhomb *Rectangle*	(hk) $(\bar{h}\bar{k})$ $(\bar{h}k)$ $(h\bar{k})$
2	*b*	*.m.*	$0, y$ $0, \bar{y}$	Pair of parallel edges *Line segment through origin*	(01) $(0\bar{1})$
2	*a*	*..m*	$x, 0$ $\bar{x}, 0$	Pair of parallel edges *Line segment through origin*	(10) $(\bar{1}0)$
1	*o*	2*mm*	$0, 0$	*Point in origin*	
SQUARE SYSTEM					
4					
4	*a*	1	x, y $\bar{x}, \bar{y}$ $\bar{y}, x$ $y, \bar{x}$	Square *Square*	(hk) $(\bar{h}\bar{k})$ $(\bar{k}h)$ $(k\bar{h})$
1	*o*	4..	$0, 0$	*Point in origin*	
4*mm*					
8	*c*	1	x, y $\bar{x}, \bar{y}$ $\bar{y}, x$ $y, \bar{x}$ $\bar{x}, y$ $x, \bar{y}$ y, x $\bar{y}, \bar{x}$	Ditetragon *Truncated square*	(hk) $(\bar{h}\bar{k})$ $(\bar{k}h)$ $(k\bar{h})$ $(\bar{h}k)$ $(h\bar{k})$ (kh) $(\bar{k}\bar{h})$
4	*b*	*..m*	x, x $\bar{x}, \bar{x}$ $\bar{x}, x$ $x, \bar{x}$	Square *Square*	(11) $(\bar{1}\bar{1})$ $(\bar{1}1)$ $(1\bar{1})$
4	*a*	*.m.*	$x, 0$ $\bar{x}, 0$ $0, x$ $0, \bar{x}$	Square *Square*	(10) $(\bar{1}0)$ (01) $(0\bar{1})$
1	*o*	4*mm*	$0, 0$	*Point in origin*	

Table 3.2.3.1 (continued)

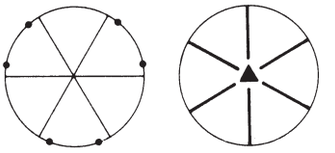
HEXAGONAL SYSTEM

3



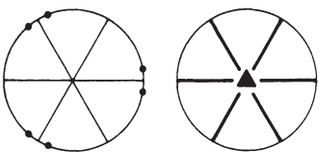
3	*a*	1	$x, y \quad \bar{y}, x-y \quad \bar{x}+y, \bar{x}$	Trigon *Trigon*	$(hki) \quad (ihk) \quad (kih)$
1	*o*	3..	0, 0	*Point in origin*	

3*m*1



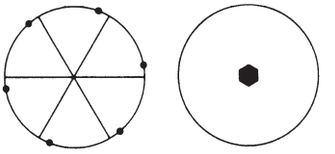
6	*b*	1	$x, y \quad \bar{y}, x-y \quad \bar{x}+y, \bar{x}$ $\bar{y}, \bar{x} \quad \bar{x}+y, y \quad x, x-y$	Ditrigon *Truncated trigon*	$(hki) \quad (ihk) \quad (kih)$ $(\bar{k}\bar{h}i) \quad (\bar{i}\bar{k}h) \quad (\bar{h}\bar{i}k)$
				Hexagon *Hexagon*	$(11\bar{2}) \quad (\bar{2}11) \quad (1\bar{2}1)$ $(\bar{1}\bar{1}2) \quad (2\bar{1}\bar{1}) \quad (\bar{1}2\bar{1})$
3	*a*	.*m*.	$x, \bar{x} \quad x, 2x \quad 2\bar{x}, \bar{x}$	Trigon *Trigon*	$(10\bar{1}) \quad (\bar{1}10) \quad (0\bar{1}1)$ or $(\bar{1}01) \quad (1\bar{1}0) \quad (01\bar{1})$
1	*o*	3*m*.	0, 0	*Point in origin*	

31*m*



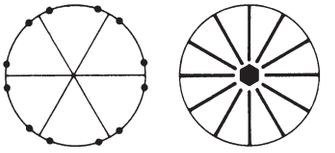
6	*b*	1	$x, y \quad \bar{y}, x-y \quad \bar{x}+y, \bar{x}$ $y, x \quad x-y, \bar{y} \quad \bar{x}, \bar{x}+y$	Ditrigon *Truncated trigon*	$(hki) \quad (ihk) \quad (kih)$ $(khi) \quad (ikh) \quad (hik)$
				Hexagon *Hexagon*	$(10\bar{1}) \quad (\bar{1}10) \quad (0\bar{1}1)$ $(01\bar{1}) \quad (\bar{1}01) \quad (1\bar{1}0)$
3	*a*	..*m*	$x, 0 \quad 0, x \quad \bar{x}, \bar{x}$	Trigon *Trigon*	$(11\bar{2}) \quad (\bar{2}11) \quad (1\bar{2}1)$ or $(\bar{1}\bar{1}2) \quad (2\bar{1}\bar{1}) \quad (\bar{1}2\bar{1})$
1	*o*	3.*m*	0, 0	*Point in origin*	

6



6	*a*	1	$x, y \quad \bar{y}, x-y \quad \bar{x}+y, \bar{x}$ $\bar{x}, \bar{y} \quad y, \bar{x}+y \quad x-y, x$	Hexagon *Hexagon*	$(hki) \quad (ihk) \quad (kih)$ $(\bar{h}\bar{k}i) \quad (\bar{i}\bar{h}k) \quad (\bar{k}\bar{i}h)$
1	*o*	6..	0, 0	*Point in origin*	

6*mm*



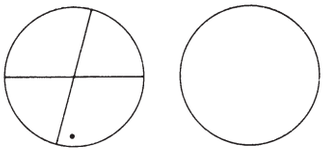
12	*c*	1	$x, y \quad \bar{y}, x-y \quad \bar{x}+y, \bar{x}$ $\bar{x}, \bar{y} \quad y, \bar{x}+y \quad x-y, x$ $\bar{y}, \bar{x} \quad \bar{x}+y, y \quad x, x-y$ $y, x \quad x-y, \bar{y} \quad \bar{x}, \bar{x}+y$	Dihexagon *Truncated hexagon*	$(hki) \quad (ihk) \quad (kih)$ $(\bar{h}\bar{k}i) \quad (\bar{i}\bar{h}k) \quad (\bar{k}\bar{i}h)$ $(\bar{k}\bar{h}i) \quad (\bar{i}\bar{k}h) \quad (\bar{h}\bar{i}k)$ $(khi) \quad (ikh) \quad (hik)$
6	*b*	.*m*.	$x, \bar{x} \quad x, 2x \quad 2\bar{x}, \bar{x}$ $\bar{x}, x \quad \bar{x}, 2\bar{x} \quad 2x, x$	Hexagon *Hexagon*	$(10\bar{1}) \quad (\bar{1}10) \quad (0\bar{1}1)$ $(\bar{1}01) \quad (1\bar{1}0) \quad (01\bar{1})$
6	*a*	..*m*	$x, 0 \quad 0, x \quad \bar{x}, \bar{x}$ $\bar{x}, 0 \quad 0, \bar{x} \quad x, x$	Hexagon *Hexagon*	$(11\bar{2}) \quad (\bar{2}11) \quad (1\bar{2}1)$ $(\bar{1}\bar{1}2) \quad (2\bar{1}\bar{1}) \quad (\bar{1}2\bar{1})$
1	*o*	6*mm*	0, 0	*Point in origin*	

Table 3.2.3.2
The 32 three-dimensional crystallographic point groups

The point groups are listed in blocks according to crystal system and are specified by their short and (if different) full Hermann–Mauguin symbols and their Schoenflies symbols. For each point group, the stereographic projections show (on the left) the general position and (on the right) the symmetry elements.
The list of Wyckoff positions includes:
Columns 1 to 4: multiplicity, Wyckoff letter, oriented site-symmetry symbol, coordinate triplets;
Under the stereographic projections: face forms (in roman type) and point forms (in italics); if there is more than one entry, subsequent entries refer to limiting (noncharacteristic) forms;
Last column: Miller indices of equivalent faces [for trigonal and hexagonal groups, Bravais–Miller indices (*hkil*) are used if referred to hexagonal axes].

TRICLINIC SYSTEM

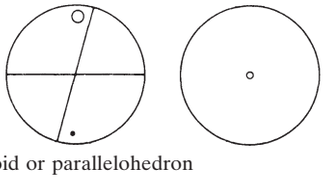
1 C_1



1	*a*	1	x, y, z	Pedion or monohedron *Single point*	(hkl)

Symmetry of special projections
Along any direction
1

$\bar{1}$ C_i

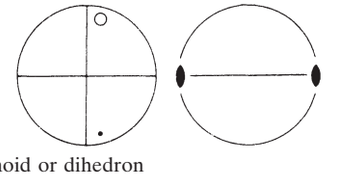


2	*a*	1	x, y, z $\bar{x}, \bar{y}, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(hkl) $(\bar{h}\bar{k}\bar{l})$
1	*o*	$\bar{1}$	0, 0, 0	*Point in origin*	

Symmetry of special projections
Along any direction
2

MONOCLINIC SYSTEM

2 UNIQUE AXIS *b* C_2

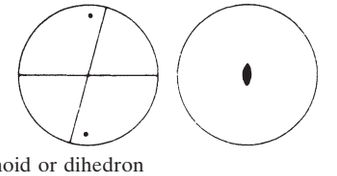


2	*b*	1	x, y, z $\bar{x}, y, \bar{z}$	Sphenoid or dihedron *Line segment*	(hkl) $(\bar{h}k\bar{l})$
				Pinacoid or parallelohedron *Line segment through origin*	$(h0l)$ $(\bar{h}0\bar{l})$
1	*a*	2	0, y, 0	Pedion or monohedron *Single point*	(010) or $(0\bar{1}0)$

Symmetry of special projections

Along [100]	Along [010]	Along [001]
m	2	*m*

2 UNIQUE AXIS *c* C_2



2	*b*	1	x, y, z $\bar{x}, \bar{y}, z$	Sphenoid or dihedron *Line segment*	(hkl) $(\bar{h}\bar{k}l)$
				Pinacoid or parallelohedron *Line segment through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$
1	*a*	2	0, 0, z	Pedion or monohedron *Single point*	(001) or $(00\bar{1})$

Symmetry of special projections

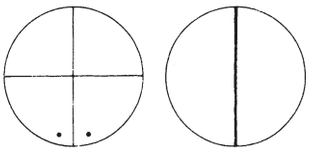
Along [100]	Along [010]	Along [001]
m	*m*	2

Table 3.2.3.2 (continued)

MONOCLINIC SYSTEM (*cont.*)

m
UNIQUE AXIS *b*

C_s



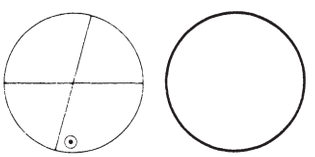
2	*b*	1	x, y, z	$x, \bar{y}, z$	Dome or dihedron *Line segment*	(hkl) $(h\bar{k}l)$
					Pinacoid or parallelohedron *Line segment through origin*	(010) $(0\bar{1}0)$
1	*a*	*m*	$x, 0, z$		Pedion or monohedron *Single point*	$(h0l)$

Symmetry of special projections

Along [100]	Along [010]	Along [001]
m	1	*m*

m
UNIQUE AXIS *c*

C_s



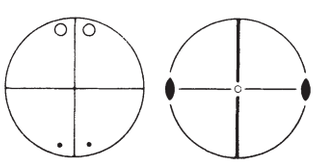
2	*b*	1	x, y, z	$x, y, \bar{z}$	Dome or dihedron *Line segment*	(hkl) $(hk\bar{l})$
					Pinacoid or parallelohedron *Line segment through origin*	(001) $(00\bar{1})$
1	*a*	*m*	$x, y, 0$		Pedion or monohedron *Single point*	$(hk0)$

Symmetry of special projections

Along [100]	Along [010]	Along [001]
m	*m*	1

2/*m*
UNIQUE AXIS *b*

C_{2h}



4	*c*	1	x, y, z	$\bar{x}, y, \bar{z}$	$\bar{x}, \bar{y}, \bar{z}$	$x, \bar{y}, z$	Rhombic prism *Rectangle through origin*	(hkl) $(\bar{h}k\bar{l})$ $(\bar{h}\bar{k}\bar{l})$ $(h\bar{k}l)$
2	*b*	*m*	$x, 0, z$	$\bar{x}, 0, \bar{z}$			Pinacoid or parallelohedron *Line segment through origin*	$(h0l)$ $(\bar{h}0\bar{l})$
2	*a*	2	$0, y, 0$	$0, \bar{y}, 0$			Pinacoid or parallelohedron *Line segment through origin*	(010) $(0\bar{1}0)$
1	*o*	2/*m*	$0, 0, 0$				*Point in origin*	

Symmetry of special projections

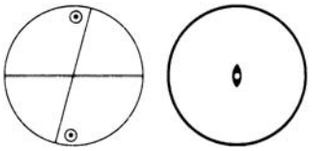
Along [100]	Along [010]	Along [001]
2*mm*	2	2*mm*

Table 3.2.3.2 (continued)

MONOCLINIC SYSTEM (*cont.*)

$2/m$ C_{2h}

UNIQUE AXIS c



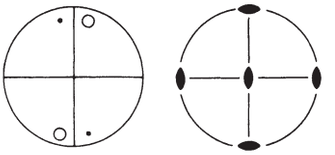
4	*c*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{x}, \bar{y}, \bar{z}$	$x, y, \bar{z}$	Rhombic prism *Rectangle through origin*	(hkl)	$(\bar{h}\bar{k}l)$	$(\bar{h}\bar{k}\bar{l})$	$(hk\bar{l})$
2	*b*	*m*	$x, y, 0$	$\bar{x}, \bar{y}, 0$			Pinacoid or parallelohedron *Line segment through origin*	$(hk0)$	$(\bar{h}\bar{k}0)$		
2	*a*	2	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron *Line segment through origin*	(001)	$(00\bar{1})$		
1	*o*	$2/m$	$0, 0, 0$				*Point in origin*				

Symmetry of special projections

Along [100]	Along [010]	Along [001]
2*mm*	2*mm*	2

ORTHORHOMBIC SYSTEM

222 D_2



4	*d*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{x}, y, \bar{z}$	$x, \bar{y}, \bar{z}$	Rhombic disphenoid or rhombic tetrahedron *Rhombic tetrahedron*	(hkl)	$(\bar{h}\bar{k}l)$	$(\bar{h}k\bar{l})$	$(h\bar{k}\bar{l})$
							Rhombic prism *Rectangle through origin*	$(hk0)$	$(\bar{h}\bar{k}0)$	$(\bar{h}k0)$	$(h\bar{k}0)$
							Rhombic prism *Rectangle through origin*	$(h0l)$	$(\bar{h}0l)$	$(\bar{h}0\bar{l})$	$(h0\bar{l})$
							Rhombic prism *Rectangle through origin*	$(0kl)$	$(0\bar{k}l)$	$(0k\bar{l})$	$(0\bar{k}\bar{l})$
2	*c*	..2	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron *Line segment through origin*	(001)	$(00\bar{1})$		
2	*b*	.2.	$0, y, 0$	$0, \bar{y}, 0$			Pinacoid or parallelohedron *Line segment through origin*	(010)	$(0\bar{1}0)$		
2	*a*	2..	$x, 0, 0$	$\bar{x}, 0, 0$			Pinacoid or parallelohedron *Line segment through origin*	(100)	$(\bar{1}00)$		
1	*o*	222	$0, 0, 0$				*Point in origin*				

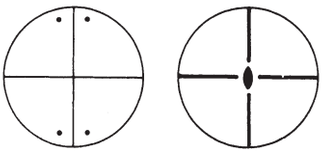
Symmetry of special projections

Along [100]	Along [010]	Along [001]
2*mm*	2*mm*	2*mm*

Table 3.2.3.2 (continued)

ORTHORHOMBIC SYSTEM (*cont.*)

$mm2$ C_{2v}

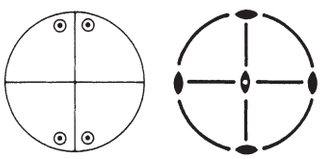


4	*d*	1	x, y, z	$\bar{x}, \bar{y}, z$	$x, \bar{y}, z$	$\bar{x}, y, z$	Rhombic pyramid *Rectangle*	(hkl)	$(\bar{h}\bar{k}l)$	$(h\bar{k}l)$	$(\bar{h}kl)$
							Rhombic prism *Rectangle through origin*	$(hk0)$	$(\bar{h}\bar{k}0)$	$(h\bar{k}0)$	$(\bar{h}k0)$
2	*c*	*m..*	$0, y, z$	$0, \bar{y}, z$			Dome or dihedron *Line segment*	$(0kl)$	$(0\bar{k}l)$		
							Pinacoid or parallelohedron *Line segment through origin*	(010)	$(0\bar{1}0)$		
2	*b*	*.m.*	$x, 0, z$	$\bar{x}, 0, z$			Dome or dihedron *Line segment*	$(h0l)$	$(\bar{h}0l)$		
							Pinacoid or parallelohedron *Line segment through origin*	(100)	$(\bar{1}00)$		
1	*a*	*mm*2	$0, 0, z$				Pedion or monohedron *Single point*	(001) or $(00\bar{1})$			

Symmetry of special projections

Along [100]	Along [010]	Along [001]
m	*m*	2*mm*

$\frac{m}{2}\frac{m}{m}\frac{m}{2}$ D_{2h}



8	*g*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{x}, y, \bar{z}$	$x, \bar{y}, \bar{z}$	Rhombic dipyramid	(hkl)	$(\bar{h}\bar{k}l)$	$(\bar{h}k\bar{l})$	$(h\bar{k}\bar{l})$
			$\bar{x}, \bar{y}, \bar{z}$	$x, y, \bar{z}$	$x, \bar{y}, z$	$\bar{x}, y, z$	*Rectangular prism*	$(\bar{h}\bar{k}\bar{l})$	$(hk\bar{l})$	$(h\bar{k}l)$	$(\bar{h}kl)$
4	*f*	*..m*	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{x}, y, 0$	$x, \bar{y}, 0$	Rhombic prism *Rectangle through origin*	$(hk0)$	$(\bar{h}\bar{k}0)$	$(\bar{h}k0)$	$(h\bar{k}0)$
4	*e*	*.m.*	$x, 0, z$	$\bar{x}, 0, z$	$\bar{x}, 0, \bar{z}$	$x, 0, \bar{z}$	Rhombic prism *Rectangle through origin*	$(h0l)$	$(\bar{h}0l)$	$(\bar{h}0\bar{l})$	$(h0\bar{l})$
4	*d*	*m..*	$0, y, z$	$0, \bar{y}, z$	$0, y, \bar{z}$	$0, \bar{y}, \bar{z}$	Rhombic prism *Rectangle through origin*	$(0kl)$	$(0\bar{k}l)$	$(0k\bar{l})$	$(0\bar{k}\bar{l})$
2	*c*	*mm*2	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron *Line segment through origin*	(001)	$(00\bar{1})$		
2	*b*	*m*2*m*	$0, y, 0$	$0, \bar{y}, 0$			Pinacoid or parallelohedron *Line segment through origin*	(010)	$(0\bar{1}0)$		
2	*a*	2*mm*	$x, 0, 0$	$\bar{x}, 0, 0$			Pinacoid or parallelohedron *Line segment through origin*	(100)	$(\bar{1}00)$		
1	*o*	*mmm*	$0, 0, 0$				*Point in origin*				

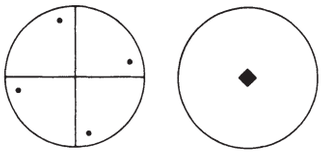
Symmetry of special projections

Along [100]	Along [010]	Along [001]
2*mm*	2*mm*	2*mm*

Table 3.2.3.2 (continued)

TETRAGONAL SYSTEM

4 C_4

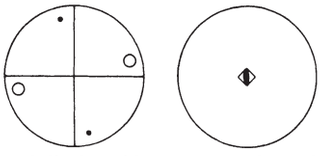


4	*b*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{y}, x, z$	$y, \bar{x}, z$	Tetragonal pyramid *Square*	(hkl)	$(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$
							Tetragonal prism *Square through origin*	$(hk0)$	$(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$
1	*a*	4..	$0, 0, z$				Pedion or monohedron *Single point*	(001) or $(00\bar{1})$	

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4	*m*	*m*

$\bar{4}$ S_4

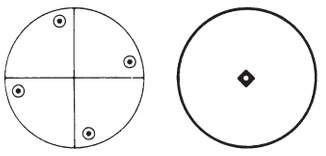


4	*b*	1	x, y, z	$\bar{x}, \bar{y}, z$	$y, \bar{x}, \bar{z}$	$\bar{y}, x, \bar{z}$	Tetragonal disphenoid or tetragonal tetrahedron *Tetragonal tetrahedron*	(hkl)	$(\bar{h}\bar{k}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$
							Tetragonal prism *Square through origin*	$(hk0)$	$(\bar{h}\bar{k}0)$ $(k\bar{h}0)$ $(\bar{k}h0)$
2	*a*	2..	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron *Line segment through origin*	(001)	$(00\bar{1})$
1	*o*	$\bar{4}$..	$0, 0, 0$				*Point in origin*		

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4	*m*	*m*

4/*m* C_{4h}



8	*c*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{y}, x, z$	$y, \bar{x}, z$	Tetragonal dipyramid	(hkl)	$(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$
			$\bar{x}, \bar{y}, \bar{z}$	$x, y, \bar{z}$	$y, \bar{x}, \bar{z}$	$\bar{y}, x, \bar{z}$	*Tetragonal prism*	$(\bar{h}\bar{k}\bar{l})$	$(hk\bar{l})$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$
4	*b*	*m*..	$x, y, 0$	$\bar{x}, \bar{y}, 0$	$\bar{y}, x, 0$	$y, \bar{x}, 0$	Tetragonal prism *Square through origin*	$(hk0)$	$(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$
2	*a*	4..	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron *Line segment through origin*	(001)	$(00\bar{1})$
1	*o*	4/*m*..	$0, 0, 0$				*Point in origin*		

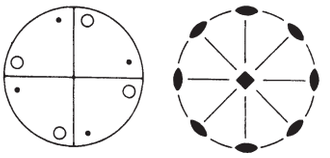
Symmetry of special projections

Along [001]	Along [100]	Along [110]
4	2*mm*	2*mm*

Table 3.2.3.2 (continued)

TETRAGONAL SYSTEM (*cont.*)

422 D_4

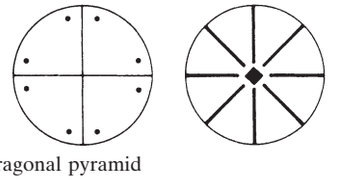


8	*d*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{y}, x, z$	$y, \bar{x}, z$	Tetragonal trapezohedron *Twisted tetragonal antiprism*	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ $(kh\bar{l})$ $(\bar{k}\bar{h}\bar{l})$
			$\bar{x}, y, \bar{z}$	$x, \bar{y}, \bar{z}$	$y, x, \bar{z}$	$\bar{y}, \bar{x}, \bar{z}$		
							Ditetragonal prism *Truncated square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$ $(\bar{h}k0)$ $(h\bar{k}0)$ $(kh0)$ $(\bar{k}\bar{h}0)$
							Tetragonal dipyramid *Tetragonal prism*	$(h0l)$ $(\bar{h}0l)$ $(0hl)$ $(0\bar{h}l)$ $(\bar{h}0\bar{l})$ $(h0\bar{l})$ $(0h\bar{l})$ $(0\bar{h}\bar{l})$
							Tetragonal dipyramid *Tetragonal prism*	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}hl)$ $(h\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ $(hh\bar{l})$ $(\bar{h}\bar{h}\bar{l})$
4	*c*	.2.	$x, 0, 0$	$\bar{x}, 0, 0$	$0, x, 0$	$0, \bar{x}, 0$	Tetragonal prism *Square through origin*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$
4	*b*	..2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$\bar{x}, x, 0$	$x, \bar{x}, 0$	Tetragonal prism *Square through origin*	(110) $(\bar{1}\bar{1}0)$ $(\bar{1}10)$ $(1\bar{1}0)$
2	*a*	4..	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron *Line segment through origin*	(001) $(00\bar{1})$
1	*o*	422	$0, 0, 0$				*Point in origin*	

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	2*mm*	2*mm*

4*mm* C_{4v}



8	*d*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{y}, x, z$	$y, \bar{x}, z$	Ditetragonal pyramid *Truncated square*	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$ $(h\bar{k}l)$ $(\bar{h}kl)$ $(\bar{k}\bar{h}l)$ (khl)
			$x, \bar{y}, z$	$\bar{x}, y, z$	$\bar{y}, \bar{x}, z$	y, x, z		
							Ditetragonal prism *Truncated square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$ $(h\bar{k}0)$ $(\bar{h}k0)$ $(\bar{k}\bar{h}0)$ $(kh0)$
4	*c*	.*m*.	$x, 0, z$	$\bar{x}, 0, z$	$0, x, z$	$0, \bar{x}, z$	Tetragonal pyramid *Square*	$(h0l)$ $(\bar{h}0l)$ $(0hl)$ $(0\bar{h}l)$
							Tetragonal prism *Square through origin*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$
4	*b*	..*m*	x, x, z	$\bar{x}, \bar{x}, z$	$\bar{x}, x, z$	$x, \bar{x}, z$	Tetragonal pyramid *Square*	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}hl)$ $(h\bar{h}l)$
							Tetragonal prism *Square through origin*	(110) $(\bar{1}\bar{1}0)$ $(\bar{1}10)$ $(1\bar{1}0)$
1	*a*	4*mm*	$0, 0, z$				Pedion or monohedron *Single point*	(001) or $(00\bar{1})$

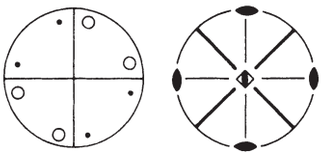
Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	*m*	*m*

Table 3.2.3.2 (continued)

TETRAGONAL SYSTEM (*cont.*)

$\bar{4}2m$ D_{2d}

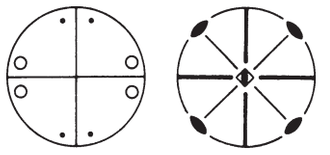


8	*d*	1	x, y, z	$\bar{x}, \bar{y}, z$	$y, \bar{x}, \bar{z}$	$\bar{y}, x, \bar{z}$	Tetragonal scalenohedron	(hkl)	$(\bar{h}\bar{k}l)$	$(k\bar{h}\bar{l})$	$(\bar{k}h\bar{l})$
			$\bar{x}, y, \bar{z}$	$x, \bar{y}, \bar{z}$	$\bar{y}, \bar{x}, z$	y, x, z	*Tetragonal tetrahedron cut off by pinacoid*	$(\bar{h}k\bar{l})$	$(h\bar{k}\bar{l})$	$(\bar{k}\bar{h}l)$	(khl)
							Ditetragonal prism	$(hk0)$	$(\bar{h}\bar{k}0)$	$(k\bar{h}0)$	$(\bar{k}h0)$
							Truncated square through origin	$(\bar{h}k0)$	$(h\bar{k}0)$	$(\bar{k}\bar{h}0)$	$(kh0)$
							Tetragonal dipyramid	$(h0l)$	$(\bar{h}0l)$	$(0\bar{h}\bar{l})$	$(0h\bar{l})$
							Tetragonal prism	$(\bar{h}0\bar{l})$	$(h0\bar{l})$	$(0\bar{h}l)$	$(0hl)$
4	*c*	..*m*	x, x, z	$\bar{x}, \bar{x}, z$	$x, \bar{x}, \bar{z}$	$\bar{x}, x, \bar{z}$	Tetragonal disphenoid or tetragonal tetrahedron	(hhl)	$(\bar{h}\bar{h}l)$	$(h\bar{h}\bar{l})$	$(\bar{h}h\bar{l})$
							Tetragonal tetrahedron				
							Tetragonal prism	(110)	$(\bar{1}\bar{1}0)$	$(1\bar{1}0)$	$(\bar{1}10)$
							Square through origin				
4	*b*	.2.	$x, 0, 0$	$\bar{x}, 0, 0$	$0, \bar{x}, 0$	$0, x, 0$	Tetragonal prism	(100)	$(\bar{1}00)$	$(0\bar{1}0)$	(010)
							Square through origin				
2	*a*	2.*mm*	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron	(001)	$(00\bar{1})$		
							Line segment through origin				
1	*o*	$\bar{4}2m$	$0, 0, 0$				*Point in origin*				

Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	2*mm*	*m*

$\bar{4}m2$ D_{2d}



8	*d*	1	x, y, z	$\bar{x}, \bar{y}, z$	$y, \bar{x}, \bar{z}$	$\bar{y}, x, \bar{z}$	Tetragonal scalenohedron	(hkl)	$(\bar{h}\bar{k}l)$	$(k\bar{h}\bar{l})$	$(\bar{k}h\bar{l})$
			$x, \bar{y}, z$	$\bar{x}, y, z$	$y, x, \bar{z}$	$\bar{y}, \bar{x}, \bar{z}$	*Tetragonal tetrahedron cut off by pinacoid*	$(h\bar{k}l)$	$(\bar{h}kl)$	$(kh\bar{l})$	$(\bar{k}\bar{h}\bar{l})$
							Ditetragonal prism	$(hk0)$	$(\bar{h}\bar{k}0)$	$(k\bar{h}0)$	$(\bar{k}h0)$
							Truncated square through origin	$(h\bar{k}0)$	$(\bar{h}k0)$	$(kh0)$	$(\bar{k}\bar{h}0)$
							Tetragonal dipyramid	(hhl)	$(\bar{h}\bar{h}l)$	$(h\bar{h}\bar{l})$	$(\bar{h}h\bar{l})$
							Tetragonal prism	$(h\bar{h}l)$	$(\bar{h}hl)$	$(hh\bar{l})$	$(\bar{h}\bar{h}\bar{l})$
4	*c*	.*m*.	$x, 0, z$	$\bar{x}, 0, z$	$0, \bar{x}, \bar{z}$	$0, x, \bar{z}$	Tetragonal disphenoid or tetragonal tetrahedron	$(h0l)$	$(\bar{h}0l)$	$(0\bar{h}\bar{l})$	$(0h\bar{l})$
							Tetragonal tetrahedron				
							Tetragonal prism	(100)	$(\bar{1}00)$	$(0\bar{1}0)$	(010)
							Square through origin				
4	*b*	..2	$x, x, 0$	$\bar{x}, \bar{x}, 0$	$x, \bar{x}, 0$	$\bar{x}, x, 0$	Tetragonal prism	(110)	$(\bar{1}\bar{1}0)$	$(1\bar{1}0)$	$(\bar{1}10)$
							Square through origin				
2	*a*	2*mm*.	$0, 0, z$	$0, 0, \bar{z}$			Pinacoid or parallelohedron	(001)	$(00\bar{1})$		
							Line segment through origin				
1	*o*	$\bar{4}m2$	$0, 0, 0$				*Point in origin*				

Symmetry of special projections

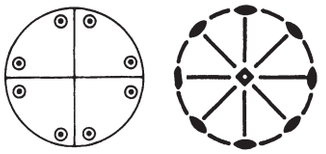
Along [001]	Along [100]	Along [110]
4*mm*	*m*	2*mm*

Table 3.2.3.2 (continued)

TETRAGONAL SYSTEM (*cont.*)

$4/mmm$

$\frac{4}{m}\frac{2}{m}\frac{2}{m}$ D_{4h}



16	*g*	1	x,y,z $\bar{x},\bar{y},z$ $\bar{y},x,z$ $y,\bar{x},z$ $\bar{x},y,\bar{z}$ $x,\bar{y},\bar{z}$ $y,x,\bar{z}$ $\bar{y},\bar{x},\bar{z}$ $\bar{x},\bar{y},\bar{z}$ $x,y,\bar{z}$ $y,\bar{x},\bar{z}$ $\bar{y},x,\bar{z}$ $x,\bar{y},z$ $\bar{x},y,z$ $\bar{y},\bar{x},z$ y,x,z	Ditetragonal dipyramid *Edge-truncated tetragonal prism*	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{k}hl)$ $(k\bar{h}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ $(kh\bar{l})$ $(\bar{k}\bar{h}\bar{l})$ $(\bar{h}\bar{k}\bar{l})$ $(hk\bar{l})$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$ $(h\bar{k}l)$ $(\bar{h}kl)$ $(\bar{k}\bar{h}l)$ (khl)
8	*f*	*.m.*	$x,0,z$ $\bar{x},0,z$ $0,x,z$ $0,\bar{x},z$ $\bar{x},0,\bar{z}$ $x,0,\bar{z}$ $0,x,\bar{z}$ $0,\bar{x},\bar{z}$	Tetragonal dipyramid *Tetragonal prism*	$(h0l)$ $(\bar{h}0l)$ $(0hl)$ $(0\bar{h}l)$ $(\bar{h}0\bar{l})$ $(h0\bar{l})$ $(0h\bar{l})$ $(0\bar{h}\bar{l})$
8	*e*	*..m*	x,x,z $\bar{x},\bar{x},z$ $\bar{x},x,z$ $x,\bar{x},z$ $\bar{x},x,\bar{z}$ $x,\bar{x},\bar{z}$ $x,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$	Tetragonal dipyramid *Tetragonal prism*	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}hl)$ $(h\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ $(hh\bar{l})$ $(\bar{h}\bar{h}\bar{l})$
8	*d*	*m..*	$x,y,0$ $\bar{x},\bar{y},0$ $\bar{y},x,0$ $y,\bar{x},0$ $\bar{x},y,0$ $x,\bar{y},0$ $y,x,0$ $\bar{y},\bar{x},0$	Ditetragonal prism *Truncated square through origin*	$(hk0)$ $(\bar{h}\bar{k}0)$ $(\bar{k}h0)$ $(k\bar{h}0)$ $(\bar{h}k0)$ $(h\bar{k}0)$ $(kh0)$ $(\bar{k}\bar{h}0)$
4	*c*	*m*2*m.*	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$	Tetragonal prism *Square through origin*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$
4	*b*	*m.m*2	$x,x,0$ $\bar{x},\bar{x},0$ $\bar{x},x,0$ $x,\bar{x},0$	Tetragonal prism *Square through origin*	(110) $(\bar{1}\bar{1}0)$ $(\bar{1}10)$ $(1\bar{1}0)$
2	*a*	4*mm*	$0,0,z$ $0,0,\bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(001) $(00\bar{1})$
1	*o*	4/*mmm*	$0,0,0$	*Point in origin*	

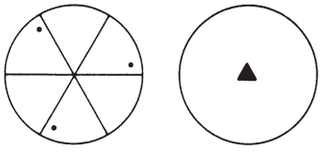
Symmetry of special projections

Along [001]	Along [100]	Along [110]
4*mm*	2*mm*	2*mm*

TRIGONAL SYSTEM

3 C_3

HEXAGONAL AXES



3	*b*	1	x,y,z $\bar{y},x-y,z$ $\bar{x}+y,\bar{x},z$	Trigonal pyramid *Trigon*	$(hkil)$ $(ihkl)$ $(kihl)$
				Trigonal prism *Trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$
1	*a*	3..	$0,0,z$	Pedion or monohedron *Single point*	(0001) or $(000\bar{1})$

Symmetry of special projections

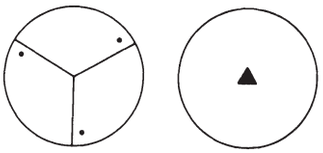
Along [001]	Along [100]	Along [210]
3	1	1

Table 3.2.3.2 (continued)

TRIGONAL SYSTEM (*cont.*)

3 C_3

RHOMBOHEDRAL AXES



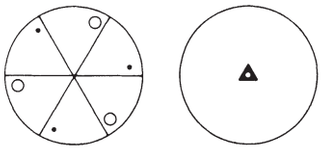
3	*b*	1	x, y, z z, x, y y, z, x	Trigonal pyramid *Trigon*	(hkl) (lhk) (klh)
				Trigonal prism *Trigon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$
1	*a*	3.	x, x, x	Pedion or monohedron *Single point*	(111) or $(\bar{1}\bar{1}\bar{1})$

Symmetry of special projections

Along [111]	Along $[1\bar{1}0]$	Along $[2\bar{1}\bar{1}]$
3	1	1

$\bar{3}$ C_{3i}

HEXAGONAL AXES



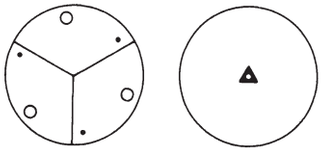
6	*b*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $\bar{x}, \bar{y}, \bar{z}$ $y, \bar{x}+y, \bar{z}$ $x-y, x, \bar{z}$	Rhombohedron *Trigonal antiprism*	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$
				Hexagonal prism *Hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$
2	*a*	3..	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) $(000\bar{1})$
1	*o*	$\bar{3}$..	$0, 0, 0$	*Point in origin*	

Symmetry of special projections

Along [001]	Along [100]	Along [210]
6	2	2

$\bar{3}$ C_{3i}

RHOMBOHEDRAL AXES



6	*b*	1	x, y, z z, x, y y, z, x $\bar{x}, \bar{y}, \bar{z}$ $\bar{z}, \bar{x}, \bar{y}$ $\bar{y}, \bar{z}, \bar{x}$	Rhombohedron *Trigonal antiprism*	(hkl) (lhk) (klh) $(\bar{h}\bar{k}\bar{l})$ $(\bar{l}\bar{h}\bar{k})$ $(\bar{k}\bar{l}\bar{h})$
				Hexagonal prism *Hexagon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$ $(\bar{h}\bar{k}(h+k))$ $((h+k)\bar{h}\bar{k})$ $(\bar{k}(h+k)\bar{h})$
2	*a*	3.	x, x, x $\bar{x}, \bar{x}, \bar{x}$	Pinacoid or parallelohedron *Line segment through origin*	(111) $(\bar{1}\bar{1}\bar{1})$
1	*o*	$\bar{3}$.	$0, 0, 0$	*Point in origin*	

Symmetry of special projections

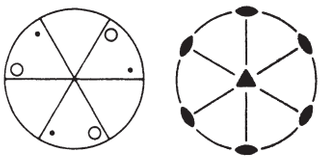
Along [111]	Along $[1\bar{1}0]$	Along $[2\bar{1}\bar{1}]$
6	2	2

Table 3.2.3.2 (continued)

TRIGONAL SYSTEM (*cont.*)

312 D_3

HEXAGONAL AXES



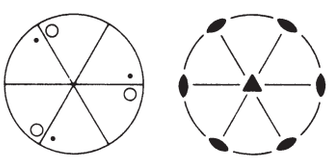
6	*c*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $\bar{y}, \bar{x}, \bar{z}$ $\bar{x}+y, y, \bar{z}$ $x, x-y, \bar{z}$	Trigonal trapezohedron *Twisted trigonal antiprism*	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{k}\bar{h}\bar{i}\bar{l})$ $(\bar{h}\bar{i}\bar{k}\bar{l})$ $(\bar{i}\bar{k}\bar{h}\bar{l})$
				Ditrigonal prism *Truncated trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
				Trigonal dipyramid *Trigonal prism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(0\bar{h}h\bar{l})$ $(\bar{h}h0\bar{l})$ $(h0\bar{h}\bar{l})$
				Rhombohedron *Trigonal antiprism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
				Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(\bar{1}2\bar{1}0)$ $(2\bar{1}\bar{1}0)$
3	*b*	..2	$x, \bar{x}, 0$ $x, 2x, 0$ $2\bar{x}, \bar{x}, 0$	Trigonal prism *Trigon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ or $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
2	*a*	3..	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) $(000\bar{1})$
1	*o*	3.2	$0, 0, 0$	*Point in origin*	

Symmetry of special projections

Along [001]	Along [100]	Along [210]
3*m*	1	2

321 D_3

HEXAGONAL AXES



6	*c*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $y, x, \bar{z}$ $x-y, \bar{y}, \bar{z}$ $\bar{x}, \bar{x}+y, \bar{z}$	Trigonal trapezohedron *Twisted trigonal antiprism*	$(hkil)$ $(ihkl)$ $(kihl)$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$
				Ditrigonal prism *Truncated trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(khi0)$ $(hik0)$ $(ikh0)$
				Trigonal dipyramid *Trigonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$
				Rhombohedron *Trigonal antiprism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$
				Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(01\bar{1}0)$ $(1\bar{1}00)$ $(\bar{1}010)$
3	*b*	.2.	$x, 0, 0$ $0, x, 0$ $\bar{x}, \bar{x}, 0$	Trigonal prism *Trigon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ or $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	3..	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) $(000\bar{1})$
1	*o*	32.	$0, 0, 0$	*Point in origin*	

Symmetry of special projections

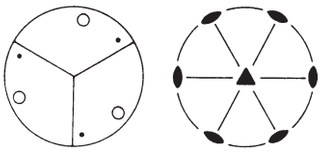
Along [001]	Along [100]	Along [210]
3*m*	2	1

Table 3.2.3.2 (continued)

TRIGONAL SYSTEM (*cont.*)

32 D_3

RHOMBOHEDRAL AXES



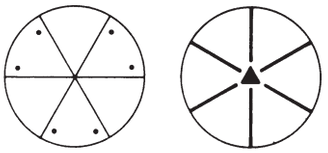
6	*c*	1	x, y, z z, x, y y, z, x $\bar{z}, \bar{y}, \bar{x}$ $\bar{y}, \bar{x}, \bar{z}$ $\bar{x}, \bar{z}, \bar{y}$	Trigonal trapezohedron *Twisted trigonal antiprism*	(hkl) (lhk) (klh) $(\bar{k}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{k})$ $(\bar{l}\bar{k}\bar{h})$
				Ditrigonal prism *Truncated trigon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$ $(\bar{k}\bar{h}(h+k))$ $(\bar{h}(h+k)\bar{k})$ $((h+k)\bar{k}\bar{h})$
				Trigonal dipyramid *Trigonal prism*	$(hk(2k-h))$ $((2k-h)hk)$ $(k(2k-h)h)$ $(\bar{k}\bar{h}(h-2k))$ $(\bar{h}(h-2k)\bar{k})$ $((h-2k)\bar{k}\bar{h})$
				Rhombohedron *Trigonal antiprism*	(hhl) (lhh) (hlh) $(\bar{h}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{h})$ $(\bar{l}\bar{h}\bar{h})$
				Hexagonal prism *Hexagon through origin*	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ $(\bar{1}\bar{1}2)$ $(\bar{1}2\bar{1})$ $(2\bar{1}\bar{1})$
3	*b*	.2	$x, \bar{x}, 0$ $0, x, \bar{x}$ $\bar{x}, 0, x$	Trigonal prism *Trigon through origin*	$(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$ or $(0\bar{1}1)$ $(10\bar{1})$ $(\bar{1}10)$
2	*a*	3.	x, x, x $\bar{x}, \bar{x}, \bar{x}$	Pinacoid or parallelohedron *Line segment through origin*	(111) $(\bar{1}\bar{1}\bar{1})$
1	*o*	32	$0, 0, 0$	*Point in origin*	

Symmetry of special projections

Along [111]	Along [1$\bar{1}$0]	Along [2$\bar{1}\bar{1}$]
3*m*	2	1

3*m*1 C_{3v}

HEXAGONAL AXES



6	*c*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $\bar{y}, \bar{x}, z$ $\bar{x}+y, y, z$ $x, x-y, z$	Ditrigonal pyramid *Truncated trigon*	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{k}\bar{h}\bar{i}l)$ $(\bar{h}\bar{i}\bar{k}l)$ $(\bar{i}\bar{k}\bar{h}l)$
				Ditrigonal prism *Truncated trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
				Hexagonal pyramid *Hexagon*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2hl)$ $(\bar{h}2h\bar{h}l)$ $(2h\bar{h}\bar{h}l)$
				Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(\bar{1}2\bar{1}0)$ $(2\bar{1}\bar{1}0)$
3	*b*	.*m*.	$x, \bar{x}, z$ $x, 2x, z$ $2\bar{x}, \bar{x}, z$	Trigonal pyramid *Trigon*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$
				Trigonal prism *Trigon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ or $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
1	*a*	3*m*.	$0, 0, z$	Pedion or monohedron *Single point*	(0001) or $(000\bar{1})$

Symmetry of special projections

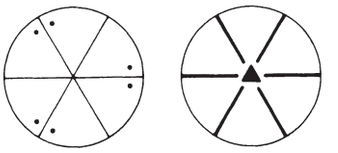
Along [001]	Along [100]	Along [210]
3*m*	1	*m*

Table 3.2.3.2 (continued)

TRIGONAL SYSTEM (*cont.*)

$31m$ C_{3v}

HEXAGONAL AXES



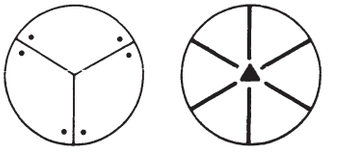
6	*c*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ y, x, z $x-y, \bar{y}, z$ $\bar{x}, \bar{x}+y, z$	Ditrigonal pyramid *Truncated trigon*	$(hkil)$ $(ihkl)$ $(kihl)$ $(khil)$ $(hikl)$ $(ikhl)$
				Ditrigonal prism *Truncated trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(khi0)$ $(hik0)$ $(ikh0)$
				Hexagonal pyramid *Hexagon*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(0h\bar{h}l)$ $(h\bar{h}0l)$ $(\bar{h}0hl)$
				Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(01\bar{1}0)$ $(1\bar{1}00)$ $(\bar{1}010)$
3	*b*	..*m*	$x, 0, z$ $0, x, z$ $\bar{x}, \bar{x}, z$	Trigonal pyramid *Trigon*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$
				Trigonal prism *Trigon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ or $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
1	*a*	3.*m*	$0, 0, z$	Pedion or monohedron *Single point*	(0001) or $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
3*m*	*m*	1

$3m$ C_{3v}

RHOMBOHEDRAL AXES



6	*c*	1	x, y, z z, x, y y, z, x z, y, x y, x, z x, z, y	Ditrigonal pyramid *Truncated trigon*	(hkl) (lhk) (klh) (khl) (hlk) (lkh)
				Ditrigonal prism *Truncated trigon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$ $(kh(\overline{h+k}))$ $(h(\overline{h+k})k)$ $((\overline{h+k})kh)$
				Hexagonal pyramid *Hexagon*	$(hk(2k-h))$ $((2k-h)hk)$ $(k(2k-h)h)$ $(kh(2k-h))$ $(h(2k-h)k)$ $((2k-h)kh)$
				Hexagonal prism *Hexagon through origin*	$(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$ $(10\bar{1})$ $(0\bar{1}1)$ $(\bar{1}10)$
3	*b*	.*m*	x, y, x x, x, y y, x, x	Trigonal pyramid *Trigon*	(hhl) (lhh) (hlh)
				Trigonal prism *Trigon through origin*	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ or $(\bar{1}\bar{1}2)$ $(2\bar{1}\bar{1})$ $(\bar{1}2\bar{1})$
1	*a*	3*m*	x, x, x	Pedion or monohedron *Single point*	(111) or $(\bar{1}\bar{1}\bar{1})$

Symmetry of special projections

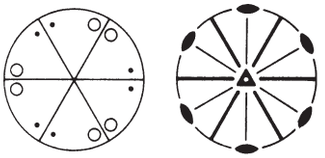
Along [111]	Along [1$\bar{1}$0]	Along [2$\bar{1}\bar{1}$]
3*m*	1	*m*

Table 3.2.3.2 (continued)

TRIGONAL SYSTEM (*cont.*)

$\bar{3}1m$
$\bar{3}1\frac{2}{m}$

D_{3d}



HEXAGONAL AXES

12	*d*	1	x, y, z	$\bar{y}, x-y, z$	$\bar{x}+y, \bar{x}, z$	Ditrigonal scalenohedron or hexagonal scalenohedron *Trigonal antiprism sliced off by pinacoid*	(*hkil*) (*ihkl*) (*kihl*) ($\bar{k}\bar{h}i\bar{l}$) ($\bar{h}\bar{i}k\bar{l}$) ($i\bar{k}\bar{h}\bar{l}$) ($\bar{h}k\bar{i}\bar{l}$) ($i\bar{h}\bar{k}l$) ($\bar{k}i\bar{h}l$) (*khil*) (*hikl*) (*ikhl*)
			$\bar{y}, \bar{x}, \bar{z}$	$\bar{x}+y, y, \bar{z}$	$x, x-y, \bar{z}$		
			$\bar{x}, \bar{y}, \bar{z}$	$y, \bar{x}+y, \bar{z}$	$x-y, x, \bar{z}$		
			y, x, z	$x-y, \bar{y}, z$	$\bar{x}, \bar{x}+y, z$		
						Dihexagonal prism *Truncated hexagon through origin*	(*hki*0) (*ihk*0) (*kih*0) ($\bar{k}\bar{h}i0$) ($\bar{h}\bar{i}k0$) ($\bar{i}\bar{k}h0$) ($\bar{h}k\bar{i}0$) ($i\bar{h}\bar{k}0$) ($\bar{k}i\bar{h}0$) (*khi*0) (*hik*0) (*ikh*0)
						Hexagonal dipyramid *Hexagonal prism*	($h0\bar{h}l$) ($\bar{h}h0l$) ($0\bar{h}hl$) ($0\bar{h}h\bar{l}$) ($\bar{h}h0\bar{l}$) ($h0\bar{h}\bar{l}$) ($\bar{h}0h\bar{l}$) ($h\bar{h}0\bar{l}$) ($0h\bar{h}\bar{l}$) ($0h\bar{h}l$) ($h\bar{h}0l$) ($\bar{h}0hl$)
6	*c*	..*m*	$x, 0, z$	$0, x, z$	$\bar{x}, \bar{x}, z$	Rhombohedron *Trigonal antiprism*	($hh\bar{2}\bar{h}l$) ($\bar{2}\bar{h}hhl$) ($h\bar{2}\bar{h}hl$) ($\bar{h}\bar{h}2h\bar{l}$) ($\bar{h}2h\bar{h}\bar{l}$) ($2h\bar{h}\bar{h}\bar{l}$)
			$0, \bar{x}, \bar{z}$	$\bar{x}, 0, \bar{z}$	$x, x, \bar{z}$		
						Hexagonal prism *Hexagon through origin*	($11\bar{2}0$) ($\bar{2}110$) ($1\bar{2}10$) ($\bar{1}\bar{1}20$) ($\bar{1}2\bar{1}0$) ($2\bar{1}\bar{1}0$)
6	*b*	..2	$x, \bar{x}, 0$	$x, 2x, 0$	$2\bar{x}, \bar{x}, 0$	Hexagonal prism *Hexagon through origin*	($10\bar{1}0$) ($\bar{1}100$) ($0\bar{1}10$) ($\bar{1}010$) ($1\bar{1}00$) ($01\bar{1}0$)
			$\bar{x}, x, 0$	$\bar{x}, 2\bar{x}, 0$	$2x, x, 0$		
2	*a*	3.*m*	$0, 0, z$	$0, 0, \bar{z}$		Pinacoid or parallelohedron *Line segment through origin*	(0001) ($000\bar{1}$)
1	*o*	$\bar{3}$.*m*	$0, 0, 0$			*Point in origin*	

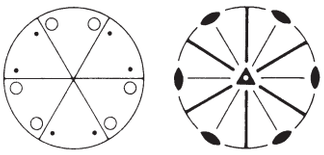
Symmetry of special projections

Along [001]	Along [100]	Along [210]
6*mm*	2*mm*	2

Table 3.2.3.2 (continued)

TRIGONAL SYSTEM (*cont.*)

$\bar{3}m1$
$\bar{3}\frac{2}{m}1$ D_{3d}



HEXAGONAL AXES

12	*d*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $y, x, \bar{z}$ $x-y, \bar{y}, \bar{z}$ $\bar{x}, \bar{x}+y, \bar{z}$ $\bar{x}, \bar{y}, \bar{z}$ $y, \bar{x}+y, \bar{z}$ $x-y, x, \bar{z}$ $\bar{y}, \bar{x}, z$ $\bar{x}+y, y, z$ $x, x-y, z$	Ditrigonal scalenohedron or hexagonal scalenohedron *Trigonal antiprism sliced off by pinacoid*	$(hkil)$ $(ihkl)$ $(kihl)$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$ $(\bar{h}\bar{k}\bar{i}\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$ $(\bar{k}\bar{h}\bar{i}l)$ $(\bar{h}\bar{i}kl)$ $(\bar{i}\bar{k}hl)$
				Dihexagonal prism *Truncated hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
				Hexagonal dipyramid *Hexagonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$ $(\bar{h}\bar{h}2h\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(\bar{h}\bar{h}2hl)$ $(\bar{h}2h\bar{h}l)$ $(2h\bar{h}\bar{h}l)$
6	*c*	.*m*.	$x, \bar{x}, z$ $x, 2x, z$ $2\bar{x}, \bar{x}, z$ $\bar{x}, x, \bar{z}$ $2x, x, \bar{z}$ $\bar{x}, 2\bar{x}, \bar{z}$	Rhombohedron *Trigonal antiprism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$
				Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(01\bar{1}0)$ $(1\bar{1}00)$ $(\bar{1}010)$
6	*b*	.2.	$x, 0, 0$ $0, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, 0, 0$ $0, \bar{x}, 0$ $x, x, 0$	Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(\bar{1}2\bar{1}0)$ $(2\bar{1}\bar{1}0)$
2	*a*	3*m*.	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) $(000\bar{1})$
1	*o*	$\bar{3}m$.	$0, 0, 0$	*Point in origin*	

Symmetry of special projections

Along [001]	Along [100]	Along [210]
6*mm*	2	2*mm*

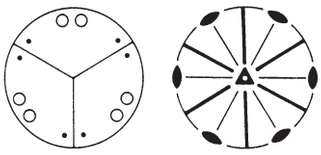
Table 3.2.3.2 (continued)

TRIGONAL SYSTEM (*cont.*)

$\bar{3}m$

$\bar{3}\frac{2}{m}$

D_{3d}



RHOMBOHEDRAL AXES

12	*d*	1	x, y, z z, x, y y, z, x $\bar{z}, \bar{y}, \bar{x}$ $\bar{y}, \bar{x}, \bar{z}$ $\bar{x}, \bar{z}, \bar{y}$ $\bar{x}, \bar{y}, \bar{z}$ $\bar{z}, \bar{x}, \bar{y}$ $\bar{y}, \bar{z}, \bar{x}$ z, y, x y, x, z x, z, y	Ditrigonal scalenohedron or hexagonal scalenohedron *Trigonal antiprism sliced off by pinacoid*	(hkl) (lhk) (klh) $(\bar{k}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{k})$ $(\bar{l}\bar{k}\bar{h})$ $(h\bar{k}\bar{l})$ $(\bar{l}h\bar{k})$ $(\bar{k}\bar{l}h)$ (khl) (hlk) (lkh)
				Dihexagonal prism *Truncated hexagon through origin*	$(hk(\overline{h+k}))$ $((\overline{h+k})hk)$ $(k(\overline{h+k})h)$ $(\bar{k}\bar{h}(h+k))$ $(\bar{h}(h+k)\bar{k})$ $((h+k)\bar{k}\bar{h})$ $(h\bar{k}(h+k))$ $((h+k)\bar{h}\bar{k})$ $(\bar{k}(h+k)\bar{h})$ $(kh(\overline{h+k}))$ $(h(\overline{h+k})k)$ $((\overline{h+k})kh)$
				Hexagonal dipyramid *Hexagonal prism*	$(hk(2k-h))$ $((2k-h)hk)$ $(k(2k-h)h)$ $(\bar{k}\bar{h}(h-2k))$ $(\bar{h}(h-2k)\bar{k})$ $((h-2k)\bar{k}\bar{h})$ $(h\bar{k}(h-2k))$ $((h-2k)\bar{h}\bar{k})$ $(\bar{k}(h-2k)\bar{h})$ $(kh(2k-h))$ $(h(2k-h)k)$ $((2k-h)kh)$
6	*c*	.*m*	x, y, x x, x, y y, x, x $\bar{x}, \bar{y}, \bar{x}$ $\bar{y}, \bar{x}, \bar{x}$ $\bar{x}, \bar{x}, \bar{y}$	Rhombohedron *Trigonal antiprism*	(hhl) (lhh) (hlh) $(\bar{h}\bar{h}\bar{l})$ $(\bar{h}\bar{l}\bar{h})$ $(\bar{l}\bar{h}\bar{h})$
				Hexagonal prism *Hexagon through origin*	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ $(\bar{1}\bar{1}2)$ $(\bar{1}2\bar{1})$ $(2\bar{1}\bar{1})$
6	*b*	.2	$x, \bar{x}, 0$ $0, x, \bar{x}$ $\bar{x}, 0, x$ $\bar{x}, x, 0$ $0, \bar{x}, x$ $x, 0, \bar{x}$	Hexagonal prism *Hexagon through origin*	$(01\bar{1})$ $(\bar{1}01)$ $(1\bar{1}0)$ $(0\bar{1}1)$ $(10\bar{1})$ $(\bar{1}10)$
2	*a*	3*m*	x, x, x $\bar{x}, \bar{x}, \bar{x}$	Pinacoid or parallelohedron *Line segment through origin*	(111) $(\bar{1}\bar{1}\bar{1})$
1	*o*	$\bar{3}m$	$0, 0, 0$	*Point in origin*	

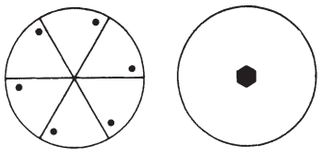
Symmetry of special projections

Along [111]	Along [1$\bar{1}$0]	Along [2$\bar{1}\bar{1}$]
6*mm*	2	2*mm*

Table 3.2.3.2 (continued)

HEXAGONAL SYSTEM

6 C_6

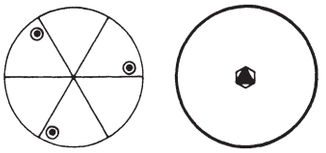


6	*b*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $\bar{x}, \bar{y}, z$ $y, \bar{x}+y, z$ $x-y, x, z$	Hexagonal pyramid *Hexagon*	(*hkil*) (*ihkl*) (*kihl*) ($\bar{h}\bar{k}$*il*) ($\bar{i}\bar{h}$*kl*) ($\bar{k}\bar{i}$*hl*)
				Hexagonal prism *Hexagon through origin*	(*hki*0) (*ihk*0) (*kih*0) ($\bar{h}\bar{k}$*i*0) ($\bar{i}\bar{h}$*k*0) ($\bar{k}\bar{i}$*h*0)
1	*a*	6..	$0, 0, z$	Pedion or monohedron *Single point*	(0001) or (000$\bar{1}$)

Symmetry of special projections

Along [001]	Along [100]	Along [210]
6	*m*	*m*

$\bar{6}$ C_{3h}

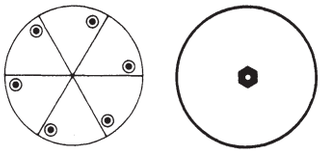


6	*c*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $x, y, \bar{z}$ $\bar{y}, x-y, \bar{z}$ $\bar{x}+y, \bar{x}, \bar{z}$	Trigonal dipyramid *Trigonal prism*	(*hkil*) (*ihkl*) (*kihl*) (*hki*$\bar{l}$) (*ihk*$\bar{l}$) (*kih*$\bar{l}$)
3	*b*	*m*..	$x, y, 0$ $\bar{y}, x-y, 0$ $\bar{x}+y, \bar{x}, 0$	Trigonal prism *Trigon through origin*	(*hki*0) (*ihk*0) (*kih*0)
2	*a*	3..	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) (000$\bar{1}$)
1	*o*	$\bar{6}$..	$0, 0, 0$	*Point in origin*	

Symmetry of special projections

Along [001]	Along [100]	Along [210]
3	*m*	*m*

6/*m* C_{6h}



12	*c*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $\bar{x}, \bar{y}, z$ $y, \bar{x}+y, z$ $x-y, x, z$ $\bar{x}, \bar{y}, \bar{z}$ $y, \bar{x}+y, \bar{z}$ $x-y, x, \bar{z}$ $x, y, \bar{z}$ $\bar{y}, x-y, \bar{z}$ $\bar{x}+y, \bar{x}, \bar{z}$	Hexagonal dipyramid *Hexagonal prism*	(*hkil*) (*ihkl*) (*kihl*) ($\bar{h}\bar{k}$*il*) ($\bar{i}\bar{h}$*kl*) ($\bar{k}\bar{i}$*hl*) (*hki*$\bar{l}$) (*ihk*$\bar{l}$) (*kih*$\bar{l}$) ($\bar{h}\bar{k}$*i*$\bar{l}$) ($\bar{i}\bar{h}$*k*$\bar{l}$) ($\bar{k}\bar{i}$*h*$\bar{l}$)
6	*b*	*m*..	$x, y, 0$ $\bar{y}, x-y, 0$ $\bar{x}+y, \bar{x}, 0$ $\bar{x}, \bar{y}, 0$ $y, \bar{x}+y, 0$ $x-y, x, 0$	Hexagonal prism *Hexagon through origin*	(*hki*0) (*ihk*0) (*kih*0) ($\bar{h}\bar{k}$*i*0) ($\bar{i}\bar{h}$*k*0) ($\bar{k}\bar{i}$*h*0)
2	*a*	6..	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) (000$\bar{1}$)
1	*o*	6/*m*..	$0, 0, 0$	*Point in origin*	

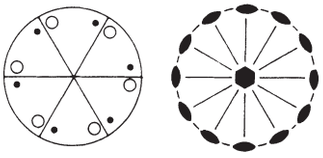
Symmetry of special projections

Along [001]	Along [100]	Along [210]
6	2*mm*	2*mm*

Table 3.2.3.2 (continued)

HEXAGONAL SYSTEM (*cont.*)

622 D_6



12	*d*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $\bar{x}, \bar{y}, z$ $y, \bar{x}+y, z$ $x-y, x, z$ $y, x, \bar{z}$ $x-y, \bar{y}, \bar{z}$ $\bar{x}, \bar{x}+y, \bar{z}$ $\bar{y}, \bar{x}, \bar{z}$ $\bar{x}+y, y, \bar{z}$ $x, x-y, \bar{z}$	Hexagonal trapezohedron *Twisted hexagonal antiprism*	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}il)$ $(\bar{i}\bar{h}kl)$ $(\bar{k}\bar{i}hl)$ $(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$ $(\bar{k}\bar{h}i\bar{l})$ $(\bar{h}\bar{i}k\bar{l})$ $(\bar{i}\bar{k}h\bar{l})$
				Dihexagonal prism *Truncated hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}i0)$ $(\bar{i}\bar{h}k0)$ $(\bar{k}\bar{i}h0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{k}\bar{h}i0)$ $(\bar{h}\bar{i}k0)$ $(\bar{i}\bar{k}h0)$
				Hexagonal dipyramid *Hexagonal prism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(\bar{h}0hl)$ $(h\bar{h}0l)$ $(0h\bar{h}l)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$ $(0\bar{h}h\bar{l})$ $(\bar{h}h0\bar{l})$ $(h0\bar{h}\bar{l})$
				Hexagonal dipyramid *Hexagonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2hl)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}2h\bar{h}l)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
6	*c*	..2	$x, \bar{x}, 0$ $x, 2x, 0$ $2\bar{x}, \bar{x}, 0$ $\bar{x}, x, 0$ $\bar{x}, 2\bar{x}, 0$ $2x, x, 0$	Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$ $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
6	*b*	.2.	$x, 0, 0$ $0, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, 0, 0$ $0, \bar{x}, 0$ $x, x, 0$	Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	6..	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) $(000\bar{1})$
1	*o*	622	$0, 0, 0$	*Point in origin*	

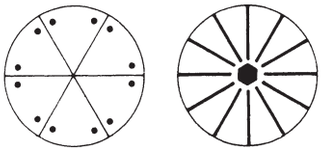
Symmetry of special projections

Along [001]	Along [100]	Along [210]
6*mm*	2*mm*	2*mm*

Table 3.2.3.2 (continued)

HEXAGONAL SYSTEM (*cont.*)

$6mm$ C_{6v}

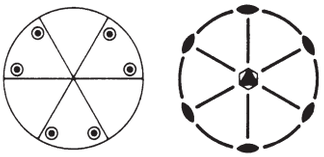


12	*d*	1	x,y,z $\bar{y},x-y,z$ $\bar{x}+y,\bar{x},z$ $\bar{x},\bar{y},z$ $y,\bar{x}+y,z$ $x-y,x,z$ $\bar{y},\bar{x},z$ $\bar{x}+y,y,z$ $x,x-y,z$ y,x,z $x-y,\bar{y},z$ $\bar{x},\bar{x}+y,z$	Dihexagonal pyramid *Truncated hexagon*	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}il)$ $(i\bar{h}\bar{k}l)$ $(\bar{k}\bar{i}hl)$ $(khil)$ $(hikl)$ $(ikhl)$ $(\bar{k}\bar{h}il)$ $(\bar{h}\bar{i}kl)$ $(\bar{i}\bar{k}hl)$
				Dihexagonal prism *Truncated hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}i0)$ $(\bar{i}\bar{h}k0)$ $(\bar{k}\bar{i}h0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{k}\bar{h}i0)$ $(\bar{h}\bar{i}k0)$ $(\bar{i}\bar{k}h0)$
6	*c*	*.m.*	$x,\bar{x},z$ $x,2x,z$ $2\bar{x},\bar{x},z$ $\bar{x},x,z$ $\bar{x},2\bar{x},z$ $2x,x,z$	Hexagonal pyramid *Hexagon*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(\bar{h}0hl)$ $(h\bar{h}0l)$ $(0h\bar{h}l)$
				Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(01\bar{1}0)$ $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
6	*b*	*..m*	$x,0,z$ $0,x,z$ $\bar{x},\bar{x},z$ $\bar{x},0,z$ $0,\bar{x},z$ x,x,z	Hexagonal pyramid *Hexagon*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2hl)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}2h\bar{h}l)$
				Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
1	*a*	$6mm$	$0,0,z$	Pedion or monohedron *Single point*	(0001) or $(000\bar{1})$

Symmetry of special projections

Along [001]	Along [100]	Along [210]
$6mm$	m	m

$\bar{6}m2$ D_{3h}



12	*e*	1	x,y,z $\bar{y},x-y,z$ $\bar{x}+y,\bar{x},z$ $x,y,\bar{z}$ $\bar{y},x-y,\bar{z}$ $\bar{x}+y,\bar{x},\bar{z}$ $\bar{y},\bar{x},z$ $\bar{x}+y,y,z$ $x,x-y,z$ $\bar{y},\bar{x},\bar{z}$ $\bar{x}+y,y,\bar{z}$ $x,x-y,\bar{z}$	Ditrigonal dipyramid *Edge-truncated trigonal prism*	$(hkil)$ $(ihkl)$ $(kihl)$ $(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$ $(\bar{k}\bar{h}il)$ $(\bar{h}\bar{i}kl)$ $(\bar{i}\bar{k}hl)$ $(\bar{k}\bar{h}i\bar{l})$ $(\bar{h}\bar{i}k\bar{l})$ $(\bar{i}\bar{k}h\bar{l})$
				Hexagonal dipyramid *Hexagonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(hh\overline{2h}\,\bar{l})$ $(\overline{2h}hh\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\bar{h}\bar{h}2hl)$ $(\bar{h}2h\bar{h}l)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
6	*d*	*m..*	$x,y,0$ $\bar{y},x-y,0$ $\bar{x}+y,\bar{x},0$ $\bar{y},\bar{x},0$ $\bar{x}+y,y,0$ $x,x-y,0$	Ditrigonal prism *Truncated trigon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{k}\bar{h}i0)$ $(\bar{h}\bar{i}k0)$ $(\bar{i}\bar{k}h0)$
				Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(\bar{1}2\bar{1}0)$ $(2\bar{1}\bar{1}0)$
6	*c*	*.m.*	$x,\bar{x},z$ $x,2x,z$ $2\bar{x},\bar{x},z$ $x,\bar{x},\bar{z}$ $x,2x,\bar{z}$ $2\bar{x},\bar{x},\bar{z}$	Trigonal dipyramid *Trigonal prism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(h0\bar{h}\bar{l})$ $(\bar{h}h0\bar{l})$ $(0\bar{h}h\bar{l})$
3	*b*	$mm2$	$x,\bar{x},0$ $x,2x,0$ $2\bar{x},\bar{x},0$	Trigonal prism *Trigon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(01\bar{1}0)$ or $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
2	*a*	*3m.*	$0,0,z$ $0,0,\bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) $(000\bar{1})$
1	*o*	$\bar{6}m2$	$0,0,0$	*Point in origin*	

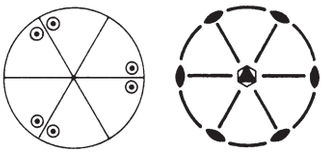
Symmetry of special projections

Along [001]	Along [100]	Along [210]
$3m$	m	$2mm$

Table 3.2.3.2 (continued)

HEXAGONAL SYSTEM (*cont.*)

$\bar{6}2m$ D_{3h}



12	*e*	1	x, y, z	$\bar{y}, x-y, z$	$\bar{x}+y, \bar{x}, z$	Ditrigonal dipyramid	$(hkil)$ $(ihkl)$ $(kihl)$
			$x, y, \bar{z}$	$\bar{y}, x-y, \bar{z}$	$\bar{x}+y, \bar{x}, \bar{z}$	*Edge-truncated trigonal prism*	$(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$
			$y, x, \bar{z}$	$x-y, \bar{y}, \bar{z}$	$\bar{x}, \bar{x}+y, \bar{z}$		$(khi\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$
			y, x, z	$x-y, \bar{y}, z$	$\bar{x}, \bar{x}+y, z$		$(khil)$ $(hikl)$ $(ikhl)$
						Hexagonal dipyramid	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$
						Hexagonal prism	$(h0\bar{h}\bar{l})$ $(\bar{h}h0\bar{l})$ $(0\bar{h}h\bar{l})$
							$(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$
							$(0h\bar{h}l)$ $(h\bar{h}0l)$ $(\bar{h}0hl)$
6	*d*	*m*..	$x, y, 0$	$\bar{y}, x-y, 0$	$\bar{x}+y, \bar{x}, 0$	Ditrigonal prism	$(hki0)$ $(ihk0)$ $(kih0)$
			$y, x, 0$	$x-y, \bar{y}, 0$	$\bar{x}, \bar{x}+y, 0$	*Truncated trigon through origin*	$(khi0)$ $(hik0)$ $(ikh0)$
						Hexagonal prism	$(10\bar{1}0)$ $(\bar{1}100)$ $(0\bar{1}10)$
						Hexagon through origin	$(01\bar{1}0)$ $(1\bar{1}00)$ $(\bar{1}010)$
6	*c*	..*m*	$x, 0, z$	$0, x, z$	$\bar{x}, \bar{x}, z$	Trigonal dipyramid	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$
			$x, 0, \bar{z}$	$0, x, \bar{z}$	$\bar{x}, \bar{x}, \bar{z}$	*Trigonal prism*	$(hh\overline{2h}\,\bar{l})$ $(\overline{2h}hh\bar{l})$ $(h\overline{2h}h\bar{l})$
3	*b*	*m*2*m*	$x, 0, 0$	$0, x, 0$	$\bar{x}, \bar{x}, 0$	Trigonal prism	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$
						Trigon through origin	or $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	3.*m*	$0, 0, z$	$0, 0, \bar{z}$		Pinacoid or parallelohedron	(0001) $(000\bar{1})$
						Line segment through origin	
1	*o*	$\bar{6}2m$	$0, 0, 0$			*Point in origin*	

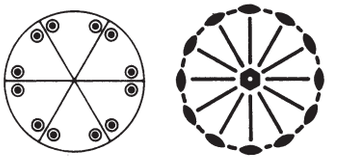
Symmetry of special projections

Along [001]	Along [100]	Along [210]
3*m*	2*mm*	*m*

Table 3.2.3.2 (continued)

HEXAGONAL SYSTEM (*cont.*)

$6/mmm$ $\quad \frac{6}{m}\frac{2}{m}\frac{2}{m}$ $\quad D_{6h}$



24	*g*	1	x, y, z $\bar{y}, x-y, z$ $\bar{x}+y, \bar{x}, z$ $\bar{x}, \bar{y}, z$ $y, \bar{x}+y, z$ $x-y, x, z$ $y, x, \bar{z}$ $x-y, \bar{y}, \bar{z}$ $\bar{x}, \bar{x}+y, \bar{z}$ $\bar{y}, \bar{x}, \bar{z}$ $\bar{x}+y, y, \bar{z}$ $x, x-y, \bar{z}$	Dihexagonal dipyramid *Edge-truncated hexagonal prism*	$(hkil)$ $(ihkl)$ $(kihl)$ $(\bar{h}\bar{k}\bar{i}\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$ $(kh\bar{i}\bar{l})$ $(hik\bar{l})$ $(ikh\bar{l})$ $(\bar{k}\bar{h}\bar{i}\,\bar{l})$ $(\bar{h}\bar{i}\bar{k}\bar{l})$ $(\bar{i}\bar{k}\bar{h}\bar{l})$
			$\bar{x}, \bar{y}, \bar{z}$ $y, \bar{x}+y, \bar{z}$ $x-y, x, \bar{z}$ $x, y, \bar{z}$ $\bar{y}, x-y, \bar{z}$ $\bar{x}+y, \bar{x}, \bar{z}$ $\bar{y}, \bar{x}, z$ $\bar{x}+y, y, z$ $x, x-y, z$ y, x, z $x-y, \bar{y}, z$ $\bar{x}, \bar{x}+y, z$		$(\bar{h}\bar{k}i\,\bar{l})$ $(\bar{i}\bar{h}\bar{k}\bar{l})$ $(\bar{k}\bar{i}\bar{h}\bar{l})$ $(hki\bar{l})$ $(ihk\bar{l})$ $(kih\bar{l})$ $(\bar{k}\bar{h}\bar{i}l)$ $(\bar{h}\bar{i}\bar{k}l)$ $(\bar{i}\bar{k}\bar{h}l)$ $(khil)$ $(hikl)$ $(ikhl)$
12	*f*	*m*..	$x, y, 0$ $\bar{y}, x-y, 0$ $\bar{x}+y, \bar{x}, 0$ $\bar{x}, \bar{y}, 0$ $y, \bar{x}+y, 0$ $x-y, x, 0$ $y, x, 0$ $x-y, \bar{y}, 0$ $\bar{x}, \bar{x}+y, 0$ $\bar{y}, \bar{x}, 0$ $\bar{x}+y, y, 0$ $x, x-y, 0$	Dihexagonal prism *Truncated hexagon through origin*	$(hki0)$ $(ihk0)$ $(kih0)$ $(\bar{h}\bar{k}\bar{i}0)$ $(\bar{i}\bar{h}\bar{k}0)$ $(\bar{k}\bar{i}\bar{h}0)$ $(khi0)$ $(hik0)$ $(ikh0)$ $(\bar{k}\bar{h}\bar{i}0)$ $(\bar{h}\bar{i}\bar{k}0)$ $(\bar{i}\bar{k}\bar{h}0)$
12	*e*	.*m*.	$x, 2x, z$ $2\bar{x}, \bar{x}, z$ $x, \bar{x}, z$ $\bar{x}, 2\bar{x}, z$ $2x, x, z$ $\bar{x}, x, z$ $2x, x, \bar{z}$ $\bar{x}, 2\bar{x}, \bar{z}$ $\bar{x}, x, \bar{z}$ $2\bar{x}, \bar{x}, \bar{z}$ $x, 2x, \bar{z}$ $x, \bar{x}, \bar{z}$	Hexagonal dipyramid *Hexagonal prism*	$(h0\bar{h}l)$ $(\bar{h}h0l)$ $(0\bar{h}hl)$ $(\bar{h}0hl)$ $(h\bar{h}0l)$ $(0h\bar{h}l)$ $(0h\bar{h}\bar{l})$ $(h\bar{h}0\bar{l})$ $(\bar{h}0h\bar{l})$ $(0\bar{h}h\bar{l})$ $(\bar{h}h0\bar{l})$ $(h0\bar{h}\bar{l})$
12	*d*	..*m*	$x, 0, z$ $0, x, z$ $\bar{x}, \bar{x}, z$ $\bar{x}, 0, z$ $0, \bar{x}, z$ x, x, z $0, x, \bar{z}$ $x, 0, \bar{z}$ $\bar{x}, \bar{x}, \bar{z}$ $0, \bar{x}, \bar{z}$ $\bar{x}, 0, \bar{z}$ $x, x, \bar{z}$	Hexagonal dipyramid *Hexagonal prism*	$(hh\overline{2h}l)$ $(\overline{2h}hhl)$ $(h\overline{2h}hl)$ $(\bar{h}\bar{h}2hl)$ $(2h\bar{h}\bar{h}l)$ $(\bar{h}2h\bar{h}l)$ $(hh\overline{2h}\bar{l})$ $(h\overline{2h}h\bar{l})$ $(\overline{2h}hh\bar{l})$ $(\bar{h}\bar{h}2h\bar{l})$ $(\bar{h}2h\bar{h}\bar{l})$ $(2h\bar{h}\bar{h}\bar{l})$
6	*c*	*mm*2	$x, 2x, 0$ $2\bar{x}, \bar{x}, 0$ $x, \bar{x}, 0$ $\bar{x}, 2\bar{x}, 0$ $2x, x, 0$ $\bar{x}, x, 0$	Hexagonal prism *Hexagon through origin*	$(10\bar{1}0)$ $(\bar{1}100)$ $(01\bar{1}0)$ $(\bar{1}010)$ $(1\bar{1}00)$ $(01\bar{1}0)$
6	*b*	*m*2*m*	$x, 0, 0$ $0, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x}, 0, 0$ $0, \bar{x}, 0$ $x, x, 0$	Hexagonal prism *Hexagon through origin*	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $(\bar{1}\bar{1}20)$ $(2\bar{1}\bar{1}0)$ $(\bar{1}2\bar{1}0)$
2	*a*	6*mm*	$0, 0, z$ $0, 0, \bar{z}$	Pinacoid or parallelohedron *Line segment through origin*	(0001) $(000\bar{1})$
1	*o*	6*mmm*	$0, 0, 0$	*Point in origin*	

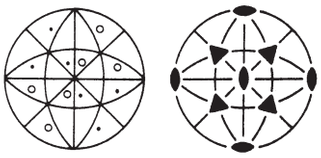
Symmetry of special projections

Along [001]	Along [100]	Along [210]
6*mm*	2*mm*	2*mm*

Table 3.2.3.2 (continued)

CUBIC SYSTEM

23 T



12	*c*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{x}, y, \bar{z}$	$x, \bar{y}, \bar{z}$	Pentagon-tritetrahedron or tetartoid	(hkl)	$(\bar{h}\bar{k}l)$	$(\bar{h}k\bar{l})$	$(h\bar{k}\bar{l})$
			z, x, y	$z, \bar{x}, \bar{y}$	$\bar{z}, \bar{x}, y$	$\bar{z}, x, \bar{y}$	or tetrahedral pentagon-dodecahedron	(lhk)	$(l\bar{h}\bar{k})$	$(\bar{l}\bar{h}k)$	$(\bar{l}h\bar{k})$
			y, z, x	$\bar{y}, z, \bar{x}$	$y, \bar{z}, \bar{x}$	$\bar{y}, \bar{z}, x$	*Snub tetrahedron* (= *pentagon-tritetrahedron* + *two tetrahedra*)	(klh)	$(\bar{k}l\bar{h})$	$(k\bar{l}\bar{h})$	$(\bar{k}\bar{l}h)$
							Trigon-tritetrahedron or tristetrahedron (for $\|h\| < \|l\|$) *Tetrahedron truncated by tetrahedron* (*for* $\|x\| < \|z\|$)	(hhl)	$(\bar{h}\bar{h}l)$	$(\bar{h}hl)$	$(h\bar{h}\bar{l})$
								(lhh)	$(l\bar{h}\bar{h})$	$(\bar{l}\bar{h}h)$	$(\bar{l}h\bar{h})$
							Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron (for $\|h\| > \|l\|$) *Cube* & *two tetrahedra* (*for* $\|x\| > \|z\|$)	(hlh)	$(\bar{h}l\bar{h})$	$(h\bar{l}\bar{h})$	$(\bar{h}\bar{l}h)$
							Pentagon-dodecahedron or dihexahedron or pyritohedron *Irregular icosahedron* (= *pentagon-dodecahedron* + *octahedron*)	$(0kl)$	$(0\bar{k}l)$	$(0k\bar{l})$	$(0\bar{k}\bar{l})$
								$(l0k)$	$(l0\bar{k})$	$(\bar{l}0k)$	$(\bar{l}0\bar{k})$
								$(kl0)$	$(\bar{k}l0)$	$(k\bar{l}0)$	$(\bar{k}\bar{l}0)$
							Rhomb-dodecahedron	(011)	$(0\bar{1}1)$	$(01\bar{1})$	$(0\bar{1}\bar{1})$
							Cuboctahedron	(101)	$(10\bar{1})$	$(\bar{1}01)$	$(\bar{1}0\bar{1})$
								(110)	$(\bar{1}10)$	$(1\bar{1}0)$	$(\bar{1}\bar{1}0)$
6	*b*	2..	$x, 0, 0$	$\bar{x}, 0, 0$			Cube or hexahedron	(100)	$(\bar{1}00)$		
			$0, x, 0$	$0, \bar{x}, 0$			*Octahedron*	(010)	$(0\bar{1}0)$		
			$0, 0, x$	$0, 0, \bar{x}$				(001)	$(00\bar{1})$		
4	*a*	.3.	x, x, x	$\bar{x}, \bar{x}, x$	$\bar{x}, x, \bar{x}$	$x, \bar{x}, \bar{x}$	Tetrahedron	(111)	$(\bar{1}\bar{1}1)$	$(\bar{1}1\bar{1})$	$(1\bar{1}\bar{1})$
							Tetrahedron	or $(\bar{1}\bar{1}\bar{1})$	$(11\bar{1})$	$(1\bar{1}1)$	$(\bar{1}11)$
1	*o*	23.	$0, 0, 0$				*Point in origin*				

Symmetry of special projections

Along [001]	Along [111]	Along [110]
2*mm*	3	*m*

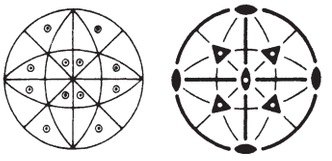
Table 3.2.3.2 (continued)

CUBIC SYSTEM (*cont.*)

$m\bar{3}$

$\frac{2}{m}\bar{3}$

T_h



24	*d*	1	x,y,z	$\bar{x},\bar{y},z$	$\bar{x},y,\bar{z}$	$x,\bar{y},\bar{z}$	Didodecahedron or diploid	(hkl)	$(\bar{h}\bar{k}l)$	$(\bar{h}k\bar{l})$	$(h\bar{k}\bar{l})$
			z,x,y	$z,\bar{x},\bar{y}$	$\bar{z},\bar{x},y$	$\bar{z},x,\bar{y}$	or dyakisdodecahedron	(lhk)	$(l\bar{h}\bar{k})$	$(\bar{l}\bar{h}k)$	$(\bar{l}h\bar{k})$
			y,z,x	$\bar{y},z,\bar{x}$	$y,\bar{z},\bar{x}$	$\bar{y},\bar{z},x$	*Cube* & *octahedron* & *pentagon-dodecahedron*	(klh)	$(\bar{k}l\bar{h})$	$(k\bar{l}\bar{h})$	$(\bar{k}\bar{l}h)$
			$\bar{x},\bar{y},\bar{z}$	$x,y,\bar{z}$	$x,\bar{y},z$	$\bar{x},y,z$		$(\bar{h}\bar{k}\bar{l})$	$(hk\bar{l})$	$(h\bar{k}l)$	$(\bar{h}kl)$
			$\bar{z},\bar{x},\bar{y}$	$\bar{z},x,y$	$z,x,\bar{y}$	$z,\bar{x},y$		$(\bar{l}\bar{h}\bar{k})$	$(\bar{l}hk)$	$(lh\bar{k})$	$(\bar{l}h\bar{k})$
			$\bar{y},\bar{z},\bar{x}$	$y,\bar{z},x$	$\bar{y},z,x$	$y,z,\bar{x}$		$(\bar{k}\bar{l}\bar{h})$	$(k\bar{l}h)$	$(\bar{k}lh)$	$(kl\bar{h})$
							Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron (for $\|h\| < \|l\|$) *Cube* & *octahedron* & *rhomb-dodecahedron* (*for* $\|x\| < \|z\|$)	(hhl)	$(\bar{h}\bar{h}l)$	$(\bar{h}h\bar{l})$	$(h\bar{h}\bar{l})$
								(lhh)	$(l\bar{h}\bar{h})$	$(\bar{l}\bar{h}h)$	$(\bar{l}h\bar{h})$
								(hlh)	$(\bar{h}l\bar{h})$	$(h\bar{l}\bar{h})$	$(\bar{h}\bar{l}h)$
							Trigon-trioctahedron or trisoctahedron (for $\|h\| > \|l\|$) *Cube truncated by octahedron* (*for* $\|x\| > \|z\|$)	$(\bar{h}\bar{h}\bar{l})$	(hhl)	$(h\bar{h}l)$	$(\bar{h}hl)$
								$(\bar{l}\bar{h}\bar{h})$	$(\bar{l}hh)$	$(lh\bar{h})$	$(\bar{l}h\bar{h})$
								$(\bar{h}\bar{l}\bar{h})$	$(h\bar{l}h)$	$(\bar{h}lh)$	$(h\bar{l}h)$
12	*c*	*m*..	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	Pentagon-dodecahedron	$(0kl)$	$(0\bar{k}l)$	$(0k\bar{l})$	$(0\bar{k}\bar{l})$
			$z,0,y$	$z,0,\bar{y}$	$\bar{z},0,y$	$\bar{z},0,\bar{y}$	or dihexahedron or pyritohedron	$(l0k)$	$(l0\bar{k})$	$(\bar{l}0k)$	$(\bar{l}0\bar{k})$
			$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$	*Irregular icosahedron* (= *pentagon-dodecahedron* + *octahedron*)	$(kl0)$	$(\bar{k}l0)$	$(k\bar{l}0)$	$(\bar{k}\bar{l}0)$
							Rhomb-dodecahedron	(011)	$(0\bar{1}1)$	$(01\bar{1})$	$(0\bar{1}\bar{1})$
							Cuboctahedron	(101)	$(10\bar{1})$	$(\bar{1}01)$	$(\bar{1}0\bar{1})$
								(110)	$(\bar{1}10)$	$(1\bar{1}0)$	$(\bar{1}\bar{1}0)$
8	*b*	.3.	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$	Octahedron	(111)	$(\bar{1}\bar{1}1)$	$(\bar{1}1\bar{1})$	$(1\bar{1}\bar{1})$
			$\bar{x},\bar{x},\bar{x}$	$x,x,\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$	*Cube*	$(\bar{1}\bar{1}\bar{1})$	$(11\bar{1})$	$(1\bar{1}1)$	$(\bar{1}11)$
6	*a*	2*mm*..	$x,0,0$	$\bar{x},0,0$			Cube or hexahedron	(100)	$(\bar{1}00)$		
			$0,x,0$	$0,\bar{x},0$			*Octahedron*	(010)	$(0\bar{1}0)$		
			$0,0,x$	$0,0,\bar{x}$				(001)	$(00\bar{1})$		
1	*o*	$m\bar{3}$.	$0,0,0$				*Point in origin*				

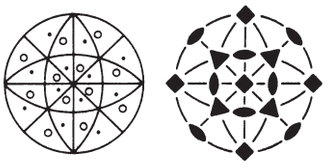
Symmetry of special projections

Along [001]	Along [111]	Along [110]
2*mm*	6	2*mm*

Table 3.2.3.2 (continued)

CUBIC SYSTEM (*cont.*)

432 O



24	*d*	1	x,y,z $\bar{x},\bar{y},z$ $\bar{x},y,\bar{z}$ $x,\bar{y},\bar{z}$ z,x,y $z,\bar{x},\bar{y}$ $\bar{z},x,\bar{y}$ $\bar{z},\bar{x},y$ y,z,x $\bar{y},z,\bar{x}$ $y,\bar{z},\bar{x}$ $\bar{y},\bar{z},x$ $y,x,\bar{z}$ $\bar{y},\bar{x},\bar{z}$ $y,\bar{x},z$ $\bar{y},x,z$ $x,z,\bar{y}$ $\bar{x},z,y$ $\bar{x},\bar{z},\bar{y}$ $x,\bar{z},y$ $z,y,\bar{x}$ $z,\bar{y},x$ $\bar{z},y,x$ $\bar{z},\bar{y},\bar{x}$	Pentagon-trioctahedron or gyroid or pentagon-icositetrahedron *Snub cube* (= *cube* + *octahedron* + *pentagon-trioctahedron*)	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ (lhk) $(l\bar{h}\bar{k})$ $(\bar{l}\bar{h}k)$ $(\bar{l}h\bar{k})$ (klh) $(\bar{k}l\bar{h})$ $(k\bar{l}\bar{h})$ $(\bar{k}\bar{l}h)$ $(kh\bar{l})$ $(\bar{k}\bar{h}\bar{l})$ $(k\bar{h}l)$ $(\bar{k}hl)$ $(hl\bar{k})$ $(\bar{h}lk)$ $(\bar{h}\bar{l}\bar{k})$ $(h\bar{l}k)$ $(lk\bar{h})$ $(l\bar{k}h)$ $(\bar{l}kh)$ $(\bar{l}\bar{k}\bar{h})$
			Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron (for $\lvert h\rvert < \lvert l\rvert$) *Cube* & *octahedron* & *rhomb-dodecahedron* (*for* $\lvert x\rvert < \lvert z\rvert$)	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ (lhh) $(l\bar{h}\bar{h})$ $(\bar{l}\bar{h}h)$ $(\bar{l}h\bar{h})$ (hlh) $(\bar{h}l\bar{h})$ $(h\bar{l}\bar{h})$ $(\bar{h}\bar{l}h)$ $(hh\bar{l})$ $(\bar{h}\bar{h}\bar{l})$ $(h\bar{h}l)$ $(\bar{h}hl)$ $(hl\bar{h})$ $(\bar{h}lh)$ $(h\bar{l}\bar{h})$ $(h\bar{l}h)$ $(lh\bar{h})$ $(l\bar{h}h)$ $(\bar{l}hh)$ $(\bar{l}\bar{h}\bar{h})$
			Trigon-trioctahedron or trisoctahedron (for $\lvert h\rvert > \lvert l\rvert$) *Cube truncated by octahedron* (*for* $\lvert x\rvert > \lvert z\rvert$)	
				$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$ $(l0k)$ $(l0\bar{k})$ $(\bar{l}0k)$ $(\bar{l}0\bar{k})$ $(kl0)$ $(\bar{k}l0)$ $(k\bar{l}0)$ $(\bar{k}\bar{l}0)$
			Tetrahexahedron or tetrakishexahedron *Octahedron truncated by cube*	$(k0l)$ $(\bar{k}0l)$ $(k0\bar{l})$ $(\bar{k}0\bar{l})$ $(0lk)$ $(0l\bar{k})$ $(0\bar{l}k)$ $(0\bar{l}\bar{k})$ $(lk0)$ $(l\bar{k}0)$ $(\bar{l}k0)$ $(\bar{l}\bar{k}0)$
12	*c*	..2	$0,y,y$ $0,\bar{y},y$ $0,y,\bar{y}$ $0,\bar{y},\bar{y}$ $y,0,y$ $y,0,\bar{y}$ $\bar{y},0,y$ $\bar{y},0,\bar{y}$ $y,y,0$ $\bar{y},y,0$ $y,\bar{y},0$ $\bar{y},\bar{y},0$	Rhomb-dodecahedron *Cuboctahedron*	(011) $(0\bar{1}1)$ $(01\bar{1})$ $(0\bar{1}\bar{1})$ (101) $(10\bar{1})$ $(\bar{1}01)$ $(\bar{1}0\bar{1})$ (110) $(\bar{1}10)$ $(1\bar{1}0)$ $(\bar{1}\bar{1}0)$
8	*b*	.3.	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x,x,\bar{x}$ $\bar{x},\bar{x},\bar{x}$ $x,\bar{x},x$ $\bar{x},x,x$	Octahedron *Cube*	(111) $(\bar{1}\bar{1}1)$ $(\bar{1}1\bar{1})$ $(1\bar{1}\bar{1})$ $(11\bar{1})$ $(\bar{1}\bar{1}\bar{1})$ $(1\bar{1}1)$ $(\bar{1}11)$
6	*a*	4..	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$	Cube or hexahedron *Octahedron*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$ (001) $(00\bar{1})$
1	*o*	432	$0,0,0$	*Point in origin*	

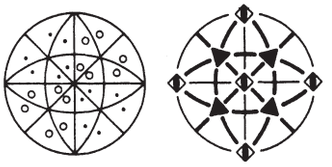
Symmetry of special projections

Along [001]	Along [111]	Along [110]
4*mm*	3*m*	2*mm*

Table 3.2.3.2 (continued)

CUBIC SYSTEM (*cont.*)

$\bar{4}3m$ T_d



24	*d*	1	x, y, z	$\bar{x}, \bar{y}, z$	$\bar{x}, y, \bar{z}$	$x, \bar{y}, \bar{z}$	Hexatetrahedron or hexakistetrahedron *Cube truncated by two tetrahedra*	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ (lhk) $(l\bar{h}\bar{k})$ $(\bar{l}\bar{h}k)$ $(\bar{l}h\bar{k})$ (klh) $(\bar{k}l\bar{h})$ $(k\bar{l}\bar{h})$ $(\bar{k}\bar{l}h)$
			z, x, y	$z, \bar{x}, \bar{y}$	$\bar{z}, \bar{x}, y$	$\bar{z}, x, \bar{y}$		
			y, z, x	$\bar{y}, z, \bar{x}$	$y, \bar{z}, \bar{x}$	$\bar{y}, \bar{z}, x$		
			y, x, z	$\bar{y}, \bar{x}, z$	$y, \bar{x}, \bar{z}$	$\bar{y}, x, \bar{z}$		(khl) $(\bar{k}\bar{h}l)$ $(k\bar{h}\bar{l})$ $(\bar{k}h\bar{l})$ (hlk) $(\bar{h}l\bar{k})$ $(h\bar{l}\bar{k})$ $(\bar{h}\bar{l}k)$ (lkh) $(l\bar{k}\bar{h})$ $(\bar{l}k\bar{h})$ $(\bar{l}\bar{k}h)$
			x, z, y	$\bar{x}, z, \bar{y}$	$\bar{x}, \bar{z}, y$	$x, \bar{z}, \bar{y}$		
			z, y, x	$z, \bar{y}, \bar{x}$	$\bar{z}, y, \bar{x}$	$\bar{z}, \bar{y}, x$		
							Tetrahexahedron or tetrakishexahedron *Octahedron truncated by cube*	$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$ $(l0k)$ $(l0\bar{k})$ $(\bar{l}0k)$ $(\bar{l}0\bar{k})$ $(kl0)$ $(\bar{k}l0)$ $(k\bar{l}0)$ $(\bar{k}\bar{l}0)$ $(k0l)$ $(\bar{k}0l)$ $(k0\bar{l})$ $(\bar{k}0\bar{l})$ $(0lk)$ $(0l\bar{k})$ $(0\bar{l}k)$ $(0\bar{l}\bar{k})$ $(lk0)$ $(l\bar{k}0)$ $(\bar{l}k0)$ $(\bar{l}\bar{k}0)$
12	*c*	..*m*	x, x, z	$\bar{x}, \bar{x}, z$	$\bar{x}, x, \bar{z}$	$x, \bar{x}, \bar{z}$	Trigon-tritetrahedron or tristetrahedron (for $\lvert h\rvert < \lvert l\rvert$) *Tetrahedron truncated by tetrahedron* (*for* $\lvert x\rvert < \lvert z\rvert$)	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ (lhh) $(l\bar{h}\bar{h})$ $(\bar{l}\bar{h}h)$ $(\bar{l}h\bar{h})$ (hlh) $(\bar{h}l\bar{h})$ $(h\bar{l}\bar{h})$ $(\bar{h}\bar{l}h)$
			z, x, x	$z, \bar{x}, \bar{x}$	$\bar{z}, \bar{x}, x$	$\bar{z}, x, \bar{x}$		
			x, z, x	$\bar{x}, z, \bar{x}$	$x, \bar{z}, \bar{x}$	$\bar{x}, \bar{z}, x$	Tetragon-tritetrahedron or deltohedron or deltoid-dodecahedron (for $\lvert h\rvert > \lvert l\rvert$) *Cube* & *two tetrahedra* (*for* $\lvert x\rvert > \lvert z\rvert$)	
							Rhomb-dodecahedron *Cuboctahedron*	(110) $(\bar{1}\bar{1}0)$ $(\bar{1}10)$ $(1\bar{1}0)$ (011) $(0\bar{1}\bar{1})$ $(0\bar{1}1)$ $(01\bar{1})$ (101) $(\bar{1}0\bar{1})$ $(10\bar{1})$ $(\bar{1}01)$
6	*b*	2.*mm*	$x, 0, 0$	$\bar{x}, 0, 0$			Cube or hexahedron *Octahedron*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$ (001) $(00\bar{1})$
			$0, x, 0$	$0, \bar{x}, 0$				
			$0, 0, x$	$0, 0, \bar{x}$				
4	*a*	.3*m*	x, x, x	$\bar{x}, \bar{x}, x$	$\bar{x}, x, \bar{x}$	$x, \bar{x}, \bar{x}$	Tetrahedron *Tetrahedron*	(111) $(\bar{1}\bar{1}1)$ $(\bar{1}1\bar{1})$ $(1\bar{1}\bar{1})$ or $(\bar{1}\bar{1}\bar{1})$ $(11\bar{1})$ $(1\bar{1}1)$ $(\bar{1}11)$
1	*o*	$\bar{4}3m$	$0, 0, 0$				*Point in origin*	

Symmetry of special projections

Along [001]	Along [111]	Along [110]
4*mm*	3*m*	*m*

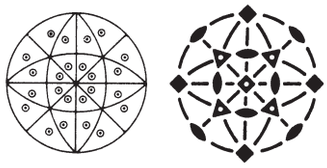
Table 3.2.3.2 (continued)

CUBIC SYSTEM (*cont.*)

$m\bar{3}m$

$\frac{4}{m}\bar{3}\frac{2}{m}$

O_h



48	*f*	1	x,y,z $\bar{x},\bar{y},z$ $\bar{x},y,\bar{z}$ $x,\bar{y},\bar{z}$ z,x,y $z,\bar{x},\bar{y}$ $\bar{z},\bar{x},y$ $\bar{z},x,\bar{y}$ y,z,x $\bar{y},z,\bar{x}$ $y,\bar{z},\bar{x}$ $\bar{y},\bar{z},x$	Hexaoctahedron or hexakisoctahedron *Cube truncated by octahedron and by rhomb-dodecahedron*	(hkl) $(\bar{h}\bar{k}l)$ $(\bar{h}k\bar{l})$ $(h\bar{k}\bar{l})$ (lhk) $(\bar{l}\bar{h}k)$ $(\bar{l}h\bar{k})$ $(l\bar{h}\bar{k})$ (klh) $(\bar{k}\bar{l}h)$ $(k\bar{l}\bar{h})$ $(\bar{k}l\bar{h})$
			$y,x,\bar{z}$ $\bar{y},\bar{x},\bar{z}$ $y,\bar{x},z$ $\bar{y},x,z$ $x,z,\bar{y}$ $\bar{x},z,y$ $\bar{x},\bar{z},\bar{y}$ $x,\bar{z},y$ $z,y,\bar{x}$ $z,\bar{y},x$ $\bar{z},y,x$ $\bar{z},\bar{y},\bar{x}$		$(k\bar{h}\bar{l})$ $(\bar{k}\bar{h}l)$ $(k\bar{h}l)$ $(\bar{k}hl)$ $(hl\bar{k})$ $(\bar{h}lk)$ $(\bar{h}l\bar{k})$ $(h\bar{l}k)$ $(lk\bar{h})$ $(l\bar{k}h)$ $(\bar{l}kh)$ $(\bar{l}\bar{k}\bar{h})$
			$\bar{x},\bar{y},\bar{z}$ $x,y,\bar{z}$ $x,\bar{y},z$ $\bar{x},y,z$ $\bar{z},\bar{x},\bar{y}$ $\bar{z},x,y$ $z,x,\bar{y}$ $z,\bar{x},y$ $\bar{y},\bar{z},\bar{x}$ $y,\bar{z},x$ $\bar{y},z,x$ $y,z,\bar{x}$		$(\bar{h}\bar{k}\bar{l})$ $(hk\bar{l})$ $(h\bar{k}l)$ $(\bar{h}kl)$ $(\bar{l}\bar{h}\bar{k})$ $(\bar{l}hk)$ $(lh\bar{k})$ $(l\bar{h}k)$ $(\bar{k}\bar{l}\bar{h})$ $(k\bar{l}h)$ $(\bar{k}lh)$ $(kl\bar{h})$
			$\bar{y},\bar{x},z$ y,x,z $\bar{y},x,\bar{z}$ $y,\bar{x},\bar{z}$ $\bar{x},\bar{z},y$ $x,\bar{z},\bar{y}$ x,z,y $\bar{x},z,\bar{y}$ $\bar{z},\bar{y},x$ $\bar{z},y,\bar{x}$ $z,\bar{y},\bar{x}$ z,y,x		$(\bar{k}\bar{h}l)$ (khl) $(\bar{k}h\bar{l})$ $(k\bar{h}\bar{l})$ $(\bar{h}\bar{l}k)$ $(h\bar{l}k)$ (hlk) $(\bar{h}lk)$ $(\bar{l}\bar{k}h)$ $(\bar{l}kh)$ $(l\bar{k}h)$ $(lk\bar{h})$
24	*e*	..*m*	x,x,z $\bar{x},\bar{x},z$ $\bar{x},x,\bar{z}$ $x,\bar{x},\bar{z}$ z,x,x $z,\bar{x},\bar{x}$ $\bar{z},\bar{x},x$ $\bar{z},x,\bar{x}$ x,z,x $\bar{x},z,\bar{x}$ $x,\bar{z},\bar{x}$ $\bar{x},\bar{z},x$	Tetragon-trioctahedron or trapezohedron or deltoid-icositetrahedron (for $\|h\| < \|l\|$) *Cube & octahedron & rhomb-dodecahedron* (*for* $\|x\| < \|z\|$)	(hhl) $(\bar{h}\bar{h}l)$ $(\bar{h}h\bar{l})$ $(h\bar{h}\bar{l})$ (lhh) $(\bar{l}\bar{h}h)$ $(\bar{l}hh)$ $(l\bar{h}\bar{h})$ (hlh) $(\bar{h}l\bar{h})$ $(h\bar{l}\bar{h})$ $(\bar{h}\bar{l}h)$
			$x,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{x},z$ $\bar{x},x,z$ $x,z,\bar{x}$ $\bar{x},z,x$ $\bar{x},\bar{z},\bar{x}$ $x,\bar{z},x$ $z,x,\bar{x}$ $z,\bar{x},x$ $\bar{z},x,x$ $\bar{z},\bar{x},\bar{x}$	Trigon-trioctahedron or trisoctahedron (for $\|h\| > \|l\|$) *Cube truncated by octahedron* (*for* $\|x\| > \|z\|$)	$(hh\bar{l})$ $(\bar{h}\bar{h}\bar{l})$ $(h\bar{h}l)$ $(\bar{h}hl)$ $(hl\bar{h})$ $(\bar{h}lh)$ $(\bar{h}l\bar{h})$ $(h\bar{l}h)$ $(lh\bar{h})$ $(\bar{l}hh)$ $(\bar{l}h\bar{h})$ $(l\bar{h}\bar{h})$
24	*d*	*m*..	$0,y,z$ $0,\bar{y},z$ $0,y,\bar{z}$ $0,\bar{y},\bar{z}$ $z,0,y$ $z,0,\bar{y}$ $\bar{z},0,y$ $\bar{z},0,\bar{y}$ $y,z,0$ $\bar{y},z,0$ $y,\bar{z},0$ $\bar{y},\bar{z},0$	Tetrahexahedron or tetrakishexahedron *Octahedron truncated by cube*	$(0kl)$ $(0\bar{k}l)$ $(0k\bar{l})$ $(0\bar{k}\bar{l})$ $(l0k)$ $(l0\bar{k})$ $(\bar{l}0k)$ $(\bar{l}0\bar{k})$ $(kl0)$ $(\bar{k}l0)$ $(k\bar{l}0)$ $(\bar{k}\bar{l}0)$
			$y,0,\bar{z}$ $\bar{y},0,\bar{z}$ $y,0,z$ $\bar{y},0,z$ $0,z,\bar{y}$ $0,z,y$ $0,\bar{z},\bar{y}$ $0,\bar{z},y$ $z,y,0$ $z,\bar{y},0$ $\bar{z},y,0$ $\bar{z},\bar{y},0$		$(k0\bar{l})$ $(\bar{k}0\bar{l})$ $(k0l)$ $(\bar{k}0l)$ $(0l\bar{k})$ $(0lk)$ $(0\bar{l}\bar{k})$ $(0\bar{l}k)$ $(lk0)$ $(l\bar{k}0)$ $(\bar{l}k0)$ $(\bar{l}\bar{k}0)$
12	*c*	*m.m*2	$0,y,y$ $0,\bar{y},y$ $0,y,\bar{y}$ $0,\bar{y},\bar{y}$ $y,0,y$ $y,0,\bar{y}$ $\bar{y},0,y$ $\bar{y},0,\bar{y}$ $y,y,0$ $\bar{y},y,0$ $y,\bar{y},0$ $\bar{y},\bar{y},0$	Rhomb-dodecahedron *Cuboctahedron*	(011) $(0\bar{1}1)$ $(01\bar{1})$ $(0\bar{1}\bar{1})$ (101) $(10\bar{1})$ $(\bar{1}01)$ $(\bar{1}0\bar{1})$ (110) $(\bar{1}10)$ $(1\bar{1}0)$ $(\bar{1}\bar{1}0)$
8	*b*	.3*m*	x,x,x $\bar{x},\bar{x},x$ $\bar{x},x,\bar{x}$ $x,\bar{x},\bar{x}$ $x,x,\bar{x}$ $\bar{x},\bar{x},\bar{x}$ $x,\bar{x},x$ $\bar{x},x,x$	Octahedron *Cube*	(111) $(\bar{1}\bar{1}1)$ $(\bar{1}1\bar{1})$ $(1\bar{1}\bar{1})$ $(11\bar{1})$ $(\bar{1}\bar{1}\bar{1})$ $(1\bar{1}1)$ $(\bar{1}11)$
6	*a*	4*m.m*	$x,0,0$ $\bar{x},0,0$ $0,x,0$ $0,\bar{x},0$ $0,0,x$ $0,0,\bar{x}$	Cube or hexahedron *Octahedron*	(100) $(\bar{1}00)$ (010) $(0\bar{1}0)$ (001) $(00\bar{1})$
1	*o*	$m\bar{3}m$	$0,0,0$	*Point in origin*	

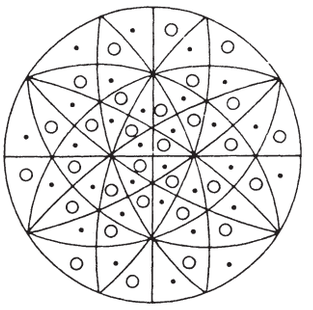
Symmetry of special projections

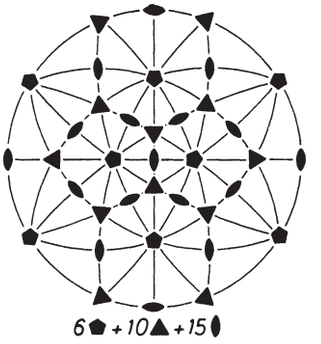
Along [001]	Along [111]	Along [110]
4*mm*	6*mm*	2*mm*

Table 3.2.3.3
The two icosahedral point groups

Each point group is specified by its Hermann–Mauguin and Schoenflies symbol. For each point group, the stereographic projections show (on the left) the general position and (on the right) the symmetry elements.
The list of the Wyckoff positions includes:
Columns 1 to 3: multiplicity, Wyckoff letter, oriented site-symmetry symbol;
Under the left stereographic projection: face forms (in roman type) and point forms (in italics), corresponding to the values for the Miller indices and coordinates listed in the last column; only 'initial' Miller indices and coordinates are given (see text).

235 *I*





60	*d*	1	Pentagon-hexecontahedron *Snub pentagon-dodecahedron* (= *pentagon-dodecahedron + icosahedron + pentagon-hexecontahedron*)	(*hkl*) *x*, *y*, *z*
			Trisicosahedron *Pentagon-dodecahedron truncated by icosahedron* (poles between axes 2 and 3)	(0*kl*) with $\|l\| < 0.382\|k\|$ 0, *y*, *z with* $\|z\| < 0.382\|y\|$
			Deltoid-hexecontahedron *Rhomb-triacontahedron* & *pentagon-dodecahedron* & *icosahedron* (poles between axes 3 and 5)	(0*kl*) with $0.382\|k\| < \|l\| < 1.618\|k\|$ 0, *y*, *z with* $0.382\|y\| < \|z\| < 1.618\|y\|$
			Pentakisdodecahedron *Icosahedron truncated by pentagon-dodecahedron* (poles between axes 5 and 2)	(0*kl*) with $\|l\| > 1.618\|k\|$ 0, *y*, *z with* $\|z\| > 1.618\|y\|$
30	*c*	2..	Rhomb-triacontahedron *Icosadodecahedron* (= *pentagon-dodecahedron* & *icosahedron*)	(100) *x*, 0, 0
20	*b*	.3.	Regular icosahedron *Regular pentagon-dodecahedron*	(111) *x*, *x*, *x*
12	*a*	..5	Regular pentagon-dodecahedron *Regular icosahedron*	(01τ) 0, *y*, τy } with $\tau = \frac{1}{2}(\sqrt{5}+1) = 1.618$
1	*o*	235	*Point in origin*	0, 0, 0

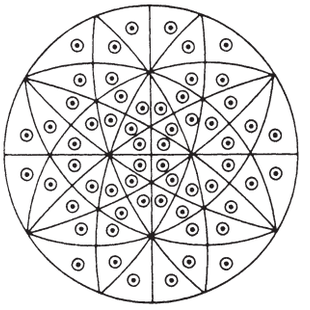
Symmetry of special projections

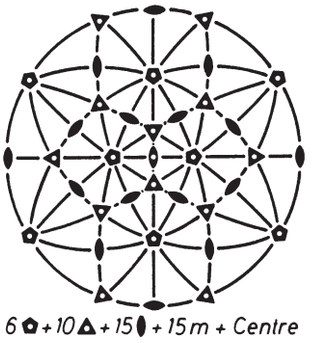
Along [001]	Along [111]	Along [1τ0]
2*mm*	3*m*	5*m*

Table 3.2.3.3 (continued)

$m\bar{3}\bar{5}$

$\frac{2}{m}\bar{3}\bar{5}$ I_h





120	*e*	1	Hecatonicosahedron or hexaicosahedron *Pentagon-dodecahedron truncated by icosahedron and by rhomb-triacontahedron*	(*hkl*) *x*, *y*, *z*
60	*d*	*m*..	Trisicosahedron *Pentagon-dodecahedron truncated by icosahedron* (poles between axes 2 and $\bar{3}$)	(0*kl*) with $\lvert l\rvert < 0.382\lvert k\rvert$ 0, *y*, *z with* $\lvert z\rvert < 0.382\lvert y\rvert$
			Deltoid-hexecontahedron *Rhomb-triacontahedron* & *pentagon-dodecahedron* & *icosahedron* (poles between axes $\bar{3}$ and $\bar{5}$)	(0*kl*) with $0.382\lvert k\rvert < \lvert l\rvert < 1.618\lvert k\rvert$ 0, *y*, *z with* $0.382\lvert y\rvert < \lvert z\rvert < 1.618\lvert y\rvert$
			Pentakisdodecahedron *Icosahedron truncated by pentagon-dodecahedron* (poles between axes $\bar{5}$ and 2)	(0*kl*) with $\lvert l\rvert > 1.618\lvert k\rvert$ 0, *y*, *z with* $\lvert z\rvert > 1.618\lvert y\rvert$
30	*c*	2*mm*..	Rhomb-triacontahedron *Icosadodecahedron* (= *pentagon-dodecahedron* & *icosahedron*)	(100) *x*, 0, 0
20	*b*	3*m* (*m*3.)	Regular icosahedron *Regular pentagon-dodecahedron*	(111) *x*, *x*, *x*
12	*a*	5*m* (*m*.5)	Regular pentagon-dodecahedron *Regular icosahedron*	(01τ) 0, *y*, τy } with $\tau = \frac{1}{2}(\sqrt{5}+1) = 1.618$
1	*o*	$2/m\bar{3}\bar{5}$	*Point in origin*	0, 0, 0

Symmetry of special projections

Along [001]	Along [111]	Along [1τ0]
2*mm*	6*mm*	10*mm*

3.2.4. Molecular symmetry

BY U. MÜLLER

3.2.4.1. Introduction

In this section, by 'molecule' we mean a separate set of closely bonded atoms; this definition includes molecular ions. The term 'molecule' as used here also includes molecular aggregates held together by hydrogen bonds or other important molecular interactions. We consider only the symmetry of isolated molecules, *i.e.* we act as if the molecule had no surroundings or a completely isotropic surrounding (even if it is a molecular ion that in reality has nearby counter ions), and we do not consider any vibrational distortions. Of course, in crystals the surroundings are not isotropic; their anisotropy is reflected in the site symmetry of the molecule. The site symmetry of the molecule in the crystal may not be higher than the molecular symmetry, and, in most cases, it is lower, *i.e.* it is a subgroup of the point group of the isolated molecule. From experience we know that the actual deviation of the molecular symmetry in crystals as compared to the symmetry in an isotropic surrounding is usually unimportant; generally, only conformation angles are affected significantly.

According to the statistical data for organic molecules (molecules having C—C or C—H bonds), the point group 1 is the most frequent (70.9%), followed by $\overline{1}$ (8.1%), 2 (7.5%), *m* (6.5%), 2/*m* (2.1%) and *mm*2 (1.7%); all others are <1% (Pidcock *et al.*, 2003). In crystals, the site symmetry of organic molecules is 1 with a frequency of 80.7%, followed by $\overline{1}$ (∼11%). Centrosymmetric molecules ($\overline{1}$ and higher centrosymmetric point groups) almost always crystallize in centrosymmetric space groups (99%) and lie on centrosymmetric sites ($\overline{1}$ and higher) with a frequency of 97% (Pidcock *et al.*, 2003; Müller, 1978).

Since all real molecules are objects of three-dimensional space, we consider only three-dimensional symmetry groups. This choice also applies to so-called 'zero-', 'one-' and 'two-dimensional' molecules; these misleading terms are sometimes used for, respectively, finite molecules, polymeric chain molecules and polymeric layer molecules. For chemists who use these terms, the 'dimensionality' mostly refers to the linkage by covalent bonds; for physicists, 'dimensionality' may refer to some other anisotropic property, *e.g.* conductivity.

3.2.4.2. Definitions

The set of all isometries that map a molecule onto itself is its *molecular symmetry*. Its symmetry operations form a group which is the *point group* $\mathcal{P}_M$ *of the molecule*.

The group $\mathcal{P}_M$ is finite if the molecule consists of a finite number of atoms and is mapped onto itself by a finite number of isometries. However, the group is infinite for linear molecules like HCl and CO_2, because of the infinite order of the molecular axis. For the symmetry of polymeric molecules see below (Section 3.2.4.4).

All symmetry operations of a finite molecule leave its centre of mass unchanged. If this point is chosen as the origin, all symmetry operations can be represented by 3×3 matrices $\boldsymbol{W}_i$, referred to some predefined coordinate system.

According to their equivalence, point groups are classified into *point-group types*. Two point groups $\mathcal{P}_{M1}$ and $\mathcal{P}_{M2}$ belong to the same *point-group type* if, after selection of appropriate coordinate systems, the matrix groups of $\mathcal{P}_{M1}$ and $\mathcal{P}_{M2}$ coincide. Why point groups and point-group types have to be distinguished is shown in the following example of metaldehyde; however, for most molecules the distinction is usually of only minor importance.

In Section 1.1.7 a general definition is given for an *orbit* under the action of a group. Applied to molecules, we formulate this definition in the following way:

The set of points symmetry-equivalent to a point X of a molecule is the *orbit of X under* $\mathcal{P}_M$.

A point X in a molecule has a definite *site symmetry* $\mathcal{S}_X$ (site-symmetry group). It consists of all those symmetry operations of the point group $\mathcal{P}_M$ which leave the point fixed. The site-symmetry group $\mathcal{S}_X$ is always a subgroup of the point group of the molecule: $\mathcal{S}_X \leq \mathcal{P}_M$.

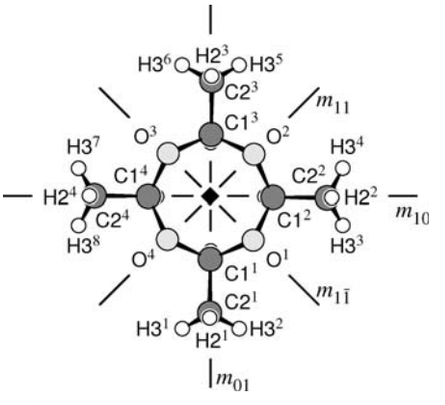
A point X is on a *general position* if its site symmetry $\mathcal{S}_X$ consists of nothing more than the identity, $\mathcal{S}_X = \mathcal{I}$. Otherwise, if $\mathcal{S}_X > \mathcal{I}$, the point is on a *special position*.

The *multiplicity* of a point X in a molecule is equal to the number of points which are symmetry-equivalent to this point, *i.e.* the number of points in its orbit. If the point is on a general position, its multiplicity is equal to the group order $|\mathcal{P}_M|$. If $|\mathcal{S}_X|$ is the order of the site symmetry of a point on a special position, the multiplicity of X is $|\mathcal{P}_M|/|\mathcal{S}_X|$.

Two points X and Y of a molecule belong to the same *Wyckoff position* if the site-symmetry groups $\mathcal{S}_X$ and $\mathcal{S}_Y$ are conjugate subgroups of $\mathcal{P}_M$, *i.e.* if $\mathcal{S}_X$ and $\mathcal{S}_Y$ are symmetry-equivalent under a symmetry operation of $\mathcal{P}_M$; expressed mathematically, this is $\mathcal{S}_Y = g\mathcal{S}_X g^{-1}$ with $g \in \mathcal{P}_M$. The special case $\mathcal{S}_X = \mathcal{S}_Y$ is included.

Example

A molecule of metaldehyde [tetrameric acetaldehyde, 2,4,6,8-tetramethyl-1,3,5,7-tetraoxacyclooctane, $(H_3CCHO)_4$] has the point group $\mathcal{P}_M = 4mm$ (C_{4v}) of order $|\mathcal{P}_M| = 8$, consisting of the symmetry operations 1, 4^+, 2, 4^-, m_{10}, m_{01}, m_{11} and $m_{1\bar{1}}$.



The atoms $C1^1 \ldots C1^4$, the four H atoms bonded to them (not labelled in the figure and largely hidden), $C2^1 \ldots C2^4$ and $H2^1 \ldots H2^4$ make up four sets of symmetry-equivalent atoms and thus form four orbits. All these atoms are placed on the mirror planes m_{10} and m_{01}; their site-symmetry groups are $\{1, m_{10}\}$ or $\{1, m_{01}\}$. $\{1, m_{10}\}$ and $\{1, m_{01}\}$ are conjugate subgroups of 4*mm* because they are equivalent by a fourfold rotation, *i.e.* $\{1, m_{01}\} = 4^+\{1, m_{10}\}4^-$. All of these atoms belong to *one* Wyckoff position, labelled 4*c* in Table 3.2.3.2. The symmetry-equivalent atoms $O^1 \ldots O^4$ make up another orbit which belongs to a different Wyckoff position, labelled 4*b*, with the conjugate site symmetries $\{1, m_{11}\}$ and $\{1, m_{1\bar{1}}\}$. Although the site symmetries of both 4*b* and 4*c* consist of the identity and one reflection, they are not conjugate because there is no symmetry operation of 4*mm* that relates them. The subgroups $\{1, m_{10}\}$ and $\{1, m_{11}\}$ are different point groups of the same point-group type.

These four site-symmetry groups all have order 2. Accordingly, the multiplicity for each of the atoms discussed above is 8/2 = 4. The atoms $H3^1 \ldots H3^8$, however, are on a general position, their site symmetry is 1 and their multiplicity corresponds to the order 8 of the point group 4*mm*. Their orbit belongs to the Wyckoff position 8*d*. The Wyckoff position 1*a* on the fourfold rotation axis is not occupied.

3.2.4.3. Tables of the point groups

In Table 3.2.3.2 all crystallographic point groups are listed, *i.e.* all point groups with axes of orders 1, 2, 3, 4 and 6. As described in Section 3.2.1.2.3, the tables also contain the crystal forms which refer to the faces of crystals. As far as molecular symmetry is concerned, only the first four columns and the names of the polyhedra (point forms) in the fifth column given in italics are of interest.

The polyhedra listed in the fifth column result when the points of one orbit of the corresponding Wyckoff position are connected by lines. As for their names, see the remarks on 'point forms' in Sections 3.2.1.2.3 and 3.2.1.2.4.

In Table 3.2.3.2 each point group is headed by its short and, if it differs, full Hermann–Mauguin symbol and by its Schoenflies symbol. Each of the subsequent entries corresponds to one Wyckoff position, in order of increasing site symmetry. The last Wyckoff position of the list is always the one with the highest site symmetry and a multiplicity of 1. The sequence of the coordinate triplets follows the sequence as for the symmorphic space groups.

The columns of Table 3.2.3.2 contain the following data:

Column 1: The multiplicity, *i.e.* the number of equivalent points.

Column 2: The Wyckoff letter, which is an alphabetical label. For all point groups with a 'floating' origin, *i.e.*, where the origin is not fixed on a unique point of highest symmetry, the last entry is the Wyckoff letter *a*. For point groups with a fixed origin, the unique origin point has the highest site symmetry and has the letter *o* (for origin).

Column 3: The site symmetry, given as an 'oriented point-group symbol' (*cf.* Section 2.1.3.12).

Column 4: Coordinates *x*, *y*, *z* of equivalent points.

Column 5: The name of the polyhedron (point form) spanned by the set of symmetry-equivalent points with the coordinates from column 4 is given in italics. The names given in roman type refer to crystal forms described in Section 3.2.1.2.3 and have no importance for molecules. In some cases, a Wyckoff position has several entries in columns 5 and 6, with several polyhedron names. All but the first one correspond to orbits of the same Wyckoff position where some special values have been assigned to one or more of the variable coordinates, *e.g.* $z = 0$, with the consequence that the eigensymmetries of these orbits are higher than the symmetry of the generating point group (non-characteristic orbits, *cf.* Section 1.4.4.4).

Since there is no lattice, point groups of molecules, unlike point groups of crystals, have no 'natural' coordinate system. It is common for coordinates of atoms in molecules to refer to a Cartesian *xyz* coordinate system; with the exception of trigonal and hexagonal point groups, the coordinates given in Table 3.2.3.2 can be taken as Cartesian coordinates with arbitrary unit length. For point groups with a floating origin, the origin 0, 0, 0 has to be assigned to an arbitrarily chosen point of the Wyckoff position 1*a*. The following conventions are used for the orientation of the coordinate axes:

Triclinic system: arbitrary orientation of the axes.

Monoclinic system: unique axis either *y* or *z*, as specified. The other two directions arbitrary but normal to the unique axis.

Orthorhombic system: Axes *x*, *y* and *z* along the symmetry directions.

Tetragonal system: *z* along the fourfold symmetry axis, *x* along the symmetry direction mentioned in the second position of the Hermann–Mauguin symbol. In the case of one-digit Hermann–Mauguin symbols the *x* direction is arbitrary within the plane normal to the unique axis. The axis *y* is normal to both *x* and *z*.

Trigonal and hexagonal systems: *z* along the unique symmetry axis, *x* along the symmetry direction mentioned second in the Hermann–Mauguin symbol. In the case of one-digit Hermann–Mauguin symbols the *x* direction is arbitrary within the plane normal to the unique axis. The axis *y* is also normal to *z*. *Note*: The coordinates given in Table 3.2.3.2 do not refer to a Cartesian, but to a symmetry-adapted coordinate system. For the hexagonal point groups and the trigonal point groups marked 'hexagonal axes' there is an angle of 120° between the *x* and *y* axes. These coordinates can be converted to a Cartesian system according to $x - \frac{1}{2}y, \frac{1}{2}\sqrt{3}y, z$. Coordinates that refer to 'rhombohedral axes' are not suited for separate molecules.

Cubic system: *x*, *y* and *z* along the symmetry directions described by the first position of the Hermann–Mauguin symbol.

For the trigonal and hexagonal systems, the following pairs of point-group types are distinguished in Table 3.2.3.2: 321 & 312, 3*m*1 & 31*m*, $\bar{3}m1$ & $\bar{3}1m$ and $\bar{6}m2$ & $\bar{6}2m$. In fact, each of these pairs represents only one molecular point-group type, the difference being only the arbitrarily chosen direction of the *x* axis. The members of each pair can be interconverted by turning the coordinate system by 30° about the *z* axis (referred to hexagonal axes). The same applies to the tetragonal pair $\bar{4}2m$ & $\bar{4}m2$, the turning angle being then 45°.

The terms triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic designate the crystal systems, *i.e.* the point groups of crystal lattices. As far as point groups of molecules are concerned, these terms only have the meaning of a classification by analogy with the crystal classes. For those who are accustomed to using Schoenflies symbols, it may seem odd to term the point groups $C_{3h} = S_3 = \bar{6}$ and $D_{3h} = \bar{6}2m$ hexagonal rather than trigonal, because the Schoenflies symbolism relies on rotoreflection operations rather than rotoinversion operations. In fact, some properties of C_{3h} and D_{3h} are rather more 'trigonal' than 'hexagonal'; for example, they have only one kind of degenerate irreducible representation (E), rather than two (E_1 and E_2) as do the other hexagonal point groups.

For the sake of treating molecular symmetries in the most uniform way, some recommendations for the preferred directions of the coordinate axes have been proposed (Joint Commission for Spectroscopy, 1955). These recommendations include:

(1) If any specifications are being made that depend on the choice of the axes (*e.g.* certain irreducible representations), the choice should explicitly be stated.

(2) For planar molecules with one three- or higher-fold axis (*z* axis): *x* axis through the greater number of atoms. For planar molecules with *mm*2 (C_{2v}) or *mmm* (D_{2h}) symmetry: *x* axis perpendicular to the plane of the molecule.

Molecular symmetry is not restricted to the crystallographic point groups. No detailed tables are given for noncrystallographic point groups, but the symbols for them can be found in Table 3.2.1.6. For the two icosahedral point groups see Section 3.2.1.4.2 and Table 3.2.3.3.

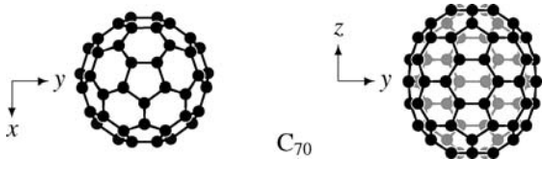
Certain physical properties depend on symmetry. In particular, a molecule can have a dipole moment only if it is polar, *i.e.* if it

has no rotoinversion axis ($\overline{2} = m$ excepted) and if it has at most one symmetry axis of order $N > 1$ and no reflection plane perpendicular to it. The polar point groups are N ($N = 1, 2, \ldots$), m, Nm (N odd) and Nmm (N even). The corresponding crystallographic point groups are those marked with a + sign under the heading 'First-rank tensor' in Table 3.2.2.1.

Examples

For the example of metaldehyde mentioned in the preceding section, we find in Table 3.2.3.2, point group 4*mm*, the Wyckoff positions 8*d*, 4*c*, 4*b* and 1*a*. Looking at the image of the molecule, we choose a coordinate system with z along the fourfold axis and x and y perpendicular to the mirror planes marked m_{10} and m_{01}. Some value has to be assigned to the unit of the (Cartesian) coordinate system, say 1 Å. The origin must be chosen at some arbitrary site on the Wyckoff position 1*a*, say such that $z = 0$ for the C1 atoms. There is no atom on the Wyckoff position 1*a* $(0, 0, z)$. The orbit consisting of the four oxygen atoms is on position 4*b* (x, x, z), $(-x, -x, z)$, $(-x, x, z)$, $(x, -x, z)$, with $x = 0.831$, $z = 0.586$; these atoms form a square and have the site symmetry *..m*, which in the image is on the mirror planes m_{11} and $m_{1\bar{1}}$. Position 4*c* $(x, 0, z)$, $(-x, 0, z)$, $(0, x, z)$, $(0, -x, z)$ has three occupied orbits: C1 with x =1.710 and (the arbitrary) $z = 0$, C2 with $x = 3.194$, $z = 0.294$ and H2; each of these orbits again forms a square and their site symmetry is *.m.* on the mirror planes m_{01} and m_{10}. The orbit of the eight H3 atoms is on the general position 8*d*; they form a truncated square. (The numerical values have been adapted from the coordinates of Barnett *et al.*, 2005).

The fullerene C_{70} is an example of a molecule with noncrystallographic symmetry, $\overline{10}\,2\,m$ (D_{5h}). This point-group type is not listed in Table 3.2.3.2, but it can be found in Table 3.2.1.6.



3.2.4.4. Polymeric molecules

Polymeric molecules actually consist of a finite number of atoms, but it is more practical to treat them as parts of infinitely extended molecules in the same way as crystals are treated as parts of ideal infinite crystals. If an infinitely long ideal molecule has translational symmetry in one direction, then its symmetry group is a rod group. If the molecule forms a layer with translational symmetry in two dimensions, its symmetry group is a layer group (not to be confused with a plane group, where space is restricted to two dimensions, *i.e.* to an infinitely thin plane).

Rod groups can have noncrystallographic symmetries, with axes of any order, such as the 10_3 screw axes in polymeric sulfur or the 29_9 axes in polyoxymethylene. Symbols for rod groups correspond to Hermann–Mauguin space-group symbols, but begin with a script style $\mathscr{h}$. The unique direction c is the direction with the translational symmetry; lattice vectors exist in this direction only and are integral multiples of **c**. This is also the direction of any rotation or screw axis with order $N > 2$. There is no natural length for the **a** and **b** vectors. If there are (twofold) rotation axes perpendicular to **c** or normals of mirror or glide planes perpendicular to **c**, these directions serve to determine the directions of **a** and **b**; otherwise, their directions are arbitrary.

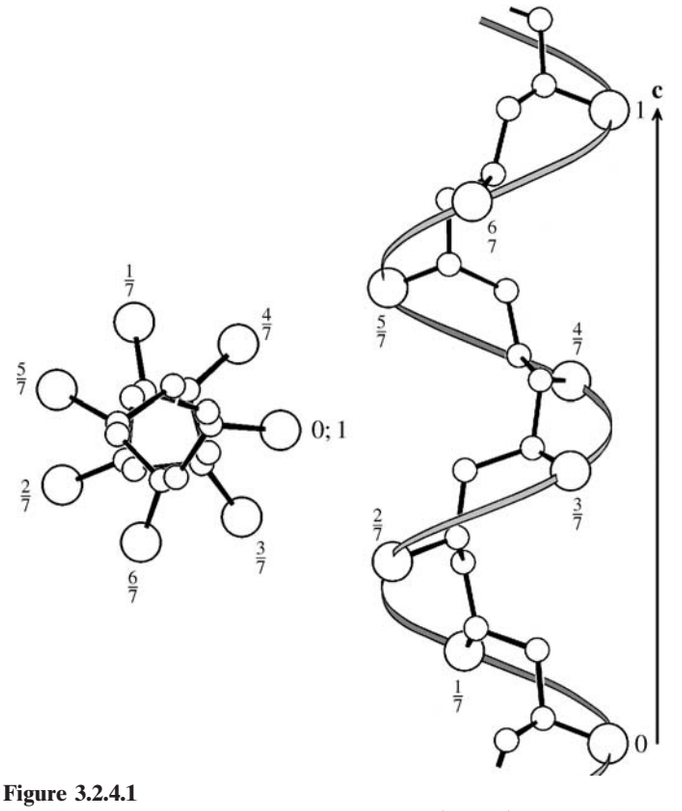


Figure 3.2.4.1
P-helix of isotactic poly-4-methyl-1-pentene (form I) with a 7/2 helix which corresponds to a 7_4 helix in Hermann–Mauguin notation. Large circles represent isobutyl groups (adapted from Natta & Corradini, 1960).

Molecules of chain polymers tend to be entangled, in which case they have no overall symmetry; symmetry is then restricted to the local symmetry in the immediate surrounding of an atom. In crystalline polymers the chains are forced to align themselves and to adopt a symmetric conformation. This symmetry can be crystallographic, but often the symmetry of the single molecule within the crystal matrix is noncrystallographic.

Crystalline chain polymers often adopt helical molecular structures. In polymer science helices are designated according to the 'helical point net system' by N/r ('N/r helix') where N is the number of repeating units within one translation period and r is the corresponding number of helical coil turns along the molecular chain (Alexander, 1969; *Compendium of Polymer Terminology and Nomenclature* (2008); Spruiell & Clark, 1980).[25] Provided that all repeating units in the chain are symmetry-equivalent, the corresponding Hermann–Mauguin screw axis symbol N_q can be calculated from

$$Nn \pm 1 = rq,$$

where n $(= 0, 1, 2, \ldots)$ and q $(0 < q < N)$ are integers to be chosen such that the equation is satisfied. The chemical handedness of the helix does not follow from the N/r symbol, but is specified by the letters M (minus; or L) and P (or R) for left and right, respectively.

Example

Isotactic poly-4-methyl-1-pentene (form I) consists of helical 7/2 chains (7 monomers per two chain windings). The equation

[25] In the IUPAC Recommendations 2011, a different notation for polymeric helices is recommended, in that a 7/2 helix be named 7_2 helix (Meille *et al.*, 2011). This is very unfortunate because it causes confusion with the Hermann–Mauguin symbols: the Hermann–Mauguin symbol of the 7/2 helix is not 7_2, but 7_4 or 7_3.

above is fulfilled either as $7 \times 1 + 1 = 2 \times 4$ or $7 \times 1 - 1 = 2 \times 3$, *i.e.* $q = 4$ or $q = 3$, and the corresponding Hermann–Mauguin screw operation symbol is either 7_4 or 7_3, depending on chirality. The helix is shown in Fig. 3.2.4.1. The *N*/*r* symbol cannot be deduced uniquely from the Hermann–Mauguin symbol, because a 7/9 or any other 7/(2 modulo 7) *P*-helix and any 7/(5 modulo 7) *M*-helix also has $\not 7_4$ symmetry.

Layer groups can have axes of orders of 1, 2, 3, 4 and 6 only. There exist 80 layer-group types. Layer-group symbols refer to a crystallographic coordinate system with **c** (of arbitrary length) perpendicular to the layer defined by the basis vectors **a** and **b**. Layer-group symbols are like space-group symbols, but begin with a lower-case *p* or *c* specifying the centring. Since plane-group symbols also begin by *p* or *c* and can therefore be confused with layer-group symbols, it is advisable to always mention what kind of group is meant.

Rod and layer groups with axis orders of 1, 2, 3, 4 and 6 are the subject of *International Tables for Crystallography* (2010), Volume E, *cf.* Section 1.7.3. Table 3.2.4.1 lists the rod-group types for any axis order.

Table 3.2.4.1
Classes of rod groups

If $N = 2$, the conventional symbols differ (the symmetry direction with the N must by shifted to the last position of the symbol and $\overline{2}$ is to be replaced by m). n is an arbitrary positive integer.

Short symbol	Full symbol	N	q
$\not N$		$N = n$	
$\not N_q$		$N = n \geq 2$	$q = 1, \ldots, N-1$
$\not \overline{N}$		$N = n$	
$\not N/m$		$N = 2n$	
$\not N_q/m$		$N = 2n$	$q = \frac{1}{2}N$
$\not N2$		$N = 2n+1$	
$\not N22$		$N = 2n$	
$\not N_q2$		$N = 2n+1$	$q = 1, \ldots, N-1$
$\not N_q22$		$N = 2n$	$q = 1, \ldots, N-1$
$\not Nm$		$N = 2n+1$	
$\not Nmm$		$N = 2n$	
$\not Nc$		$N = 2n+1$	
$\not Ncc$		$N = 2n$	
$\not N_qmc$		$N = 2n$	$q = \frac{1}{2}N$
$\not \overline{N}m$	$\not \overline{N}2/m$	$N = 2n+1$	
$\not \overline{N}2m$		$N = 2n$	
$\not \overline{N}c$	$\not \overline{N}2/c$	$N = 2n+1$	
$\not \overline{N}2c$		$N = 2n$	
$\not N/mmm$	$\not N/m2/m2/m$	$N = 2n$	
$\not N/mcc$	$\not N/m2/c2/c$	$N = 2n$	
$\not N_q/mmc$	$\not N_q/m2/m2/c$	$N = 2n$	$q = \frac{1}{2}N$

3.2.4.5. Enantiomorphism and chirality

Definition: An object is *chiral* if it cannot be superposed by pure rotation and translation on its image formed by inversion through a point.

The symmetry group of a chiral object contains no symmetry operations of the second kind, *i.e.* no inversion, rotoinversion, reflection or glide reflection. As a consequence, a chiral object can occur in two different forms, which are related in the same way as are a right and a left hand. Further terms in this context are (Flack, 2003; Moss, 1996):

Absolute configuration	Spatial arrangement of atoms in a chiral molecule and its appropriate designation [*e.g.* by (*R*), (*S*) *etc*.]
Absolute (crystal) structure	Spatial arrangement of atoms in a chiral crystal and its description (lattice parameters, space group, atomic coordinates)
Enantiomorph	One out of a pair of objects of opposite chirality
Enantiomer	One molecule out of a pair of opposite chirality (special designation for enantiomorphic molecules)
Racemate	Equimolar mixture of a pair of enantiomers
Chirality sense (chirality)	Property which distinguishes enantiomorphs from one another; the two enantiomorphs of a pair have opposite chirality
Achiral	Refers to an object that is not chiral

Possible point groups for chiral molecules correspond to the crystal classes marked in Table 3.2.2.1 with a + sign under the heading 'Enantiomorphism'. In addition, the noncrystallographic point groups N, $N2$ (N odd, $N \geq 5$), $N22$ (N even, $N \geq 8$) and 235 are possible. Chiral crystal structures are compatible only with space groups that have no inversion centres, rotoinversion axes, reflection or glide-reflection planes. For a chiral molecular compound, these symmetry elements would generate the opposite enantiomer and the compound would be a racemate. Chiral crystals belong to one of the 11 crystal classes allowing enantiomorphism (Table 3.2.2.1); they can adopt one out of 65 space-group types. These are called the 65 *Sohncke space-group types* [after L. Sohncke who was the first to derive them; Flack (2003). Julian (2015) calls them 'proper space groups']. The Sohncke space-group types comprise the eleven pairs of enantiomorphic space-group types (*cf.* Section 1.3.4.1) and further 43 non-enantiomorphic space-group types. Whereas an enantiomorphic space group (*e.g.* $P3_1$ or $P4_122$) is chiral in itself, which means that its Euclidean normalizer is noncentrosymmetric, the space groups of the other 43 Sohncke space-group types (*e.g.* $P2_12_12_1$) are not chiral themselves; they have centrosymmetric Euclidean normalizers. Keep in mind that the symmetry of a molecule is specified by its point group; the symmetry of a crystal by its space group; and the symmetry of a space group by its Euclidean normalizer (*cf.* Section 3.5.1.2).[26] However, the arrangement of the atoms in any Sohncke space group is always chiral. In other words, an enantiomorphic space group is a sufficient but not a necessary condition for a chiral crystal structure. Chirality in a non-chiral space group results if the molecules or other building blocks of the crystal consist of only one kind of enantiomers or because the molecules or building blocks, without having to be chiral themselves, are arranged in a chiral manner in the crystal.

Examples

Trigonal selenium exhibits two enantiomorphic forms that consist of either right-handed or left-handed helical chain molecules (rod groups $\not 3_12$ and $\not 3_22$, respectively). The molecules as well as the space groups $P3_121$ and $P3_221$ are enantiomorphic and the helical molecules of right-handed

[26] Many structural researchers are not aware of the difference between chiral (enantiomorphic) space groups and Sohncke space groups; frequently, even in textbooks, the term 'chiral space group' is used although an achiral Sohncke space group is meant.

selenium are incompatible with the space group of left-handed selenium.

The case of selenium can be contrasted to that of NaP (details for NaP are given at the end of Section 3.5.3.2 in the *Example for case 1*). Crystalline NaP contains one kind of enantiomeric, helical $(P^-)_\infty$ ions that are either 4_1 or 4_3 helices (rod groups $\not\!\!P4_122$ and $\not\!\!P4_322$, respectively). In this case the space group $P2_12_12_1$ is a non-enantiomorphic (achiral) Sohncke space group. It is therefore compatible with either of the two different NaP enantiomorphs.

The building blocks of $NaClO_3$, namely spherical Na^+ ions and pyramidal ClO_3^- ions (point group $3m$), are not chiral, but their arrangement in the crystal is chiral. Both enantiomorphs adopt the same non-enantiomorphic Sohncke space group $P2_13$ (Abrahams & Bernstein, 1977; Bruke-Laing & Trueblood, 1977).

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3.3. Space-group symbols and their use

H. Burzlaff and H. Zimmermann

3.3.1. Point-group symbols

3.3.1.1. Introduction

For symbolizing space groups, or more correctly types of space groups, different notations have been proposed. The following three are the main ones in use today:

(i) the notation of Schoenflies (1891, 1923);

(ii) the notation of Shubnikov (Shubnikov & Koptsik, 1972), which is frequently used in the Russian literature;

(iii) the international notation of Hermann (1928*a*) and Mauguin (1931). This was used in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (*IT* 1935) and was somewhat modified in *International Tables for X-ray Crystallography* (*IT* 1952).

In all three notations, the space-group symbol is a modification of a point-group symbol.

Symmetry elements occur in lattices, and thus in crystals, only in distinct directions. Point-group symbols make use of these discrete directions and their mutual relations.

3.3.1.2. Schoenflies symbols

Most Schoenflies symbols (Table 3.3.1.3, column 1) consist of the basic parts C_n, D_n,[1] T or O, designating cyclic, dihedral, tetrahedral and octahedral rotation groups, respectively, with $n = 1, 2, 3, 4, 6$. The remaining point groups are described by additional symbols for mirror planes, if present. The subscripts h and v indicate mirror planes perpendicular and parallel to a main axis taken as vertical. For T, the three mutually perpendicular twofold axes and, for O, the three fourfold axes are considered to be the main axes. The index d is used for mirror planes that bisect the angle between two consecutive equivalent rotation axes, *i.e.* which are diagonal with respect to these axes. For the rotoinversion axes $\overline{1}$, $\overline{2} \equiv m$, $\overline{3}$ and $\overline{4}$, which do not fit into the general Schoenflies concept of symbols, other symbols C_i, C_s, C_{3i} and S_4 are in use. The rotoinversion axis $\overline{6}$ is equivalent to $3/m$ and thus designated as C_{3h}.

A detailed introduction to Schoenflies symbols of crystallographic point groups is given in Section 1.4.1.3.

3.3.1.3. Shubnikov symbols

The Shubnikov symbol is constructed from a minimal set of generators of a point group (for exceptions, see below). Thus, strictly speaking, the symbols represent types of symmetry operations. Since each symmetry operation is related to a symmetry element, the symbols also have a geometrical meaning. The Shubnikov symbols for symmetry operations differ slightly from the international symbols (Table 3.3.1.1). Note that Shubnikov, like Schoenflies, regards symmetry operations of the second kind as rotoreflections rather than as rotoinversions.

If more than one generator is required, it is not sufficient to give only the types of the symmetry elements; their mutual orientations must be symbolized too. In the Shubnikov symbol, a dot (·), a colon (:) or a slash (/) is used to designate parallel, perpendicular or oblique arrangement of the symmetry elements. For a reflection, the orientation of the actual mirror plane is considered, not that of its normal. The exception mentioned above is the use of $3 : m$ instead of $\tilde{3}$ in the description of point groups.

[1] Instead of D_2, in older papers V (from *Vierergruppe*) is used.

3.3.1.4. Hermann–Mauguin symbols

3.3.1.4.1. Symmetry directions

The Hermann–Mauguin symbols for finite point groups make use of the fact that the symmetry elements, *i.e.* proper and improper rotation axes, have definite mutual orientations. If for each point group the symmetry directions are grouped into classes of symmetry equivalence, at most three classes are obtained. These classes were called *Blickrichtungssysteme* (Heesch, 1929). If a class contains more than one direction, one of them is chosen as representative.

The Hermann–Mauguin symbols for the crystallographic point groups refer to the symmetry directions of the lattice point groups (holohedries, *cf.* Sections 1.3.4.3 and 3.1.1.4) and use other representatives than chosen by Heesch [*IT* (1935), p. 13]. For instance, in the hexagonal case, the primary set of lattice symmetry directions consists of $\{[001], [00\overline{1}]\}$, representative is [001]; the secondary set of lattice symmetry directions consists of [100], [010], $[\overline{1}10]$ and their counter-directions, representative is [100]; the tertiary set of lattice symmetry directions consists of $[1\overline{1}0]$, [120], $[\overline{2}10]$ and their counter-directions, representative is $[1\overline{1}0]$. The representatives for the sets of lattice symmetry directions for all lattice point groups are listed in Table 3.3.1.2. The directions are related to the conventional crystallographic basis of each lattice point group (*cf.* Section 3.1.1.4).

The relation between the concept of lattice symmetry directions and group theory is evident. The maximal cyclic subgroups of the maximal rotation group contained in a lattice point group can be divided into, at most, three sets of conjugate subgroups. Each of these sets corresponds to one set of lattice symmetry directions.

Table 3.3.1.1
International (Hermann–Mauguin) and Shubnikov symbols for symmetry elements

The first power of a symmetry operation is often designated by the symmetry-element symbol without exponent 1, the other powers of the operation carry the appropriate exponent.

	Symmetry elements	
	of the first kind	of the second kind
Hermann–Mauguin	1 2 3 4 6	$\bar{1}$ m $\bar{3}$ $\bar{4}$ $\bar{6}$
Shubnikov†	1 2 3 4 6	$\tilde{2}$ m $\tilde{6}$ $\tilde{4}$ $\tilde{3}$

† According to a private communication from J. D. H. Donnay, the symbols for elements of the second kind were proposed by M. J. Buerger. Koptsik (1966) used them for the Shubnikov method.

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Table 3.3.1.2
Representatives for the sets of lattice symmetry directions in the various crystal families

	Crystal family	Anorthic (triclinic)	Monoclinic	Orthorhombic	Tetragonal	Hexagonal		Cubic
Lattice point group	Schoenflies	C_i	C_{2h}	D_{2h}	D_{4h}	D_{6h}	D_{3d}	O_h
	Hermann–Mauguin	$\bar{1}$	$\frac{2}{m}$	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	$\bar{3}\frac{2}{m}$†	$\frac{4}{m}\bar{3}\frac{2}{m}$
Set of lattice symmetry directions	Primary	–	[010] *b* unique [001] *c* unique	[100]	[001]	[001]	[001]	[001]
	Secondary	–	–	[010]	[100]	[100]	[100]	[111]
	Tertiary	–	–	[001]	[1$\bar{1}$0]	[1$\bar{1}$0]	–	[1$\bar{1}$0] [110]‡

† In this table, the directions refer to the hexagonal description. The use of the primitive rhombohedral cell brings out the relations between cubic and rhombohedral groups: the primary set is represented by [111] and the secondary by [1$\bar{1}$0]. ‡ Only for $\bar{4}3m$ and 432 [for reasons see text].

3.3.1.4.2. Full Hermann–Mauguin symbols

After the classification of the directions of rotation axes, the description of the seven maximal rotation subgroups of the lattice point groups is rather simple. For each representative direction, the rotational symmetry element is symbolized by an integer n for an n-fold axis, resulting in the symbols of the maximal rotation subgroups 1, 2, 222, 32, 422, 622, 432. The symbol 1 is used for the triclinic case. The complete lattice point group is constructed by multiplying the rotation group by the inversion $\bar{1}$. For the even-fold axes, 2, 4 and 6, this multiplication results in a mirror plane perpendicular to the rotation axis yielding the symbols $(2n)/m$ (n = 1, 2, 3). For the odd-fold axes 1 and 3, this product leads to the rotoinversion axes $\bar{1}$ and $\bar{3}$. Thus, for each representative of a set of lattice symmetry directions, the symmetry forms a point group that can be generated by one, or at most two, symmetry operations. The resulting symbols are called *full Hermann–Mauguin (or international) symbols*. For the lattice point groups they are shown in Table 3.3.1.2.

For the description of a point group of a crystal, we use its lattice symmetry directions. For the representative of each set of lattice symmetry directions, the remaining subgroup is symbolized; if only the primary symmetry direction contains symmetry higher than 1, the symbols '1' for the secondary and tertiary set (if present) can be omitted. For the cubic point groups T and T_h, the representative of the tertiary set would be '1', which is omitted. For the rotoinversion groups $\bar{1}$ and $\bar{3}$, the remaining subgroups can only be 1 and 3. If the supergroup is $(2n)/m$, five different types of subgroups can be derived: n/m, $2n$, $\overline{2n}$, n and m. In the cubic system, for instance, $4/m$, $2/m$, $\bar{4}$, 4 or 2 may occur in the primary set. In this case, the symbol m can only occur in the combinations $2/m$ or $4/m$ as can be seen from Table 3.3.1.3.

3.3.1.4.3. Short symbols and generators

If the symbols are not only used for the identification of a group but also for its construction, the symbol must contain a list of generating operations and additional relations, if necessary. Following this aspect, the Hermann–Mauguin symbols can be shortened. The choice of generators is not unique; two proposals were presented by Mauguin (1931). In the first proposal, in almost all cases the generators are the same as those of the Shubnikov symbols. In the second proposal, which, apart from some exceptions (see Section 3.3.4), is used for the international symbols, Mauguin selected a set of generators and thus a list of short symbols in which reflections have priority (Table 3.3.1.3, column 3). This selection makes the transition from the short point-group symbols to the space-group symbols fairly simple. These short symbols contain two kinds of notation components:

Table 3.3.1.3
Point-group symbols

Schoenflies	Shubnikov	*International Tables*, short symbol	*International Tables*, full symbol
C_1	1	1	1
C_i	$\tilde{2}$	$\bar{1}$	$\bar{1}$
C_2	2	2	2
C_s	m	m	m
C_{2h}	2 : m	$2/m$	$2/m$
D_2	2 : 2	222	222
C_{2v}	2 · m	$mm2$	$mm2$
D_{2h}	m · 2 : m	mmm	$2/m\ 2/m\ 2/m$
C_4	4	4	4
S_4	$\tilde{4}$	$\bar{4}$	$\bar{4}$
C_{4h}	4 : m	$4/m$	$4/m$
D_4	4 : 2	422	422
C_{4v}	4 · m	$4mm$	$4mm$
D_{2d}	$\tilde{4}$: 2	$\bar{4}2m$ or $\bar{4}m2$	$\bar{4}2m$ or $\bar{4}m2$
D_{4h}	m · 4 : m	$4/mmm$	$4/m\ 2/m\ 2/m$
C_3	3	3	3
C_{3i}	$\tilde{6}$	$\bar{3}$	$\bar{3}$
D_3	3 : 2	32 or 321 or 312	32 or 321 or 312
C_{3v}	3 · m	$3m$ or $3m1$ or $31m$	$3m$ or $3m1$ or $31m$
D_{3d}	$\tilde{6}$ · m	$\bar{3}m$ or $\bar{3}m1$ or $\bar{3}1m$	$\bar{3}\ 2/m$ or $\bar{3}\ 2/m1$ or $\bar{3}12/m$
C_6	6	6	6
C_{3h}	3 : m	$\bar{6}$	$\bar{6}$
C_{6h}	6 : m	$6/m$	$6/m$
D_6	6 : 2	622	622
C_{6v}	6 · m	$6mm$	$6mm$
D_{3h}	m · 3 : m	$\bar{6}m2$ or $\bar{6}2m$	$\bar{6}m2$ or $\bar{6}2m$
D_{6h}	m · 6 : m	$6/mmm$	$6/m\ 2/m\ 2/m$
T	3/2	23	23
T_h	$\tilde{6}/2$	$m\bar{3}$	$2/m\bar{3}$
O	3/4	432	432
T_d	$3/\tilde{4}$	$\bar{4}3m$	$\bar{4}3m$
O_h	$\tilde{6}/4$	$m\bar{3}m$	$4/m\ \bar{3}\ 2/m$

(i) components that represent the type of the generating operation, which are called *generators*;
(ii) components that are not used as generators but that serve to fix the directions of other symmetry elements (Hermann, 1931), and which are called *indicators*.

The generating matrices are uniquely defined by (i) and (ii) if it is assumed that they describe motions with counterclockwise rotational sense about the representative direction looked at end on by the observer. The symbols 2, 4, $\bar{4}$, 6 and $\bar{6}$ referring to direction [001] are indicators when the point-group symbol uses three sets of lattice symmetry directions. For instance, in 4*mm* the indicator 4 fixes the directions of the mirrors normal to [100] and [1$\bar{1}$0].

Note: The generation of (*a*) point group 432 by a rotation 3 around [111] and a rotation 2 and (*b*) point group $\bar{4}3m$ by 3 around [111] and a reflection *m* is only possible if the representative direction of the tertiary set is changed from [1$\bar{1}$0] to [110]; otherwise only the subgroup 32 or 3*m* of 432 or $\bar{4}3m$ will be generated.

Table 3.3.2.1
Symbols of glide planes in the Shubnikov and Hermann–Mauguin space-group symbols

Glide plane perpendicular to	Glide vector	Shubnikov symbol	Hermann–Mauguin symbol
b or **c**	$\frac{1}{2}\mathbf{a}$	$\tilde{a}$	*a*
a or **c**	$\frac{1}{2}\mathbf{b}$	$\tilde{b}$	*b*
a or **b** or **a** − **b**	$\frac{1}{2}\mathbf{c}$	$\tilde{c}$	*c*
c	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\widetilde{ab}$	*n*
a	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$	$\widetilde{bc}$	*n*
b	$\frac{1}{2}(\mathbf{c}+\mathbf{a})$	$\widetilde{ac}$	*n*
a − **b**	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\widetilde{abc}$	*n*
c	$\frac{1}{4}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}\widetilde{ab}$	*d*
a	$\frac{1}{4}(\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{bc}$	*d*
b	$\frac{1}{4}(\mathbf{c}+\mathbf{a})$	$\frac{1}{2}\widetilde{ac}$	*d*
a − **b**	$\frac{1}{4}(\mathbf{a}+\mathbf{b}+\mathbf{c})$	$\frac{1}{2}\widetilde{abc}$	*d*
a + **b**	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$		*d*

3.3.2. Space-group symbols

3.3.2.1. Introduction

Each space group is related to a crystallographic point group. Space-group symbols, therefore, can be obtained by a modification of point-group symbols. The simplest modification which merely gives an enumeration of the space-group types (*cf.* Section 1.3.4.1) has been used by Schoenflies. The Shubnikov and Hermann–Mauguin symbols, however, reveal the glide or screw components of the symmetry operations and are designed in such a way that the nature of the symmetry elements and their relative locations can be deduced from the symbol. [A detailed discussion and listings of computer-adapted space-group symbols implemented in crystallographic software, such as the so-called *Hall symbols* (Hall, 1981*a*,*b*) or *explicit symbols* (Shmueli, 1984), can be found in Chapter 1.4 of *International Tables for Crystallography*, Volume B (2008).]

3.3.2.2. Schoenflies symbols

Space groups related to one point group are distinguished by adding a numerical superscript to the point-group symbol. Thus, the space groups related to the point group C_2 are called C_2^1, C_2^2, C_2^3.

3.3.2.3. The role of translation parts in the Shubnikov and Hermann–Mauguin symbols

A crystallographic symmetry operation W (*cf.* Chapter 1.2) is described by a pair of matrices

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{w})(\boldsymbol{W}, \boldsymbol{o}).$$

$\boldsymbol{W}$ is called the *rotation part*, $\boldsymbol{w}$ describes the *translation part* and determines the translation vector **w** of the operation. The translation part $\boldsymbol{w}$ can be decomposed into a *glide/screw part* $\boldsymbol{w}_g$ and a *location part* $\boldsymbol{w}_l$: $\boldsymbol{w} = \boldsymbol{w}_g + \boldsymbol{w}_l$; here, $\boldsymbol{w}_l$ determines the location of the corresponding symmetry element with respect to the origin. The glide/screw part $\boldsymbol{w}_g$ may be derived by projecting $\boldsymbol{w}$ on the space invariant under $\boldsymbol{W}$, *i.e.* for rotations and reflections $\boldsymbol{w}$ is projected on the corresponding rotation axis or mirror plane. With matrix notation, $\boldsymbol{w}_g$ is determined by $(\boldsymbol{W}, \boldsymbol{w})^k = (\boldsymbol{I}, \boldsymbol{t})$ and $\boldsymbol{w}_g = (m/k)\boldsymbol{t}_1$, where k is the order of $\boldsymbol{W}$, the integers m are restricted by $0 \leq m < k$ and $\boldsymbol{t}_1$ is the shortest lattice vector in the direction of $\boldsymbol{t}$ (for details, *cf.* Sections 1.2.2.4 and 1.5.4.1). Space groups contain sets of screw and rotation axes or glide and mirror planes. A screw rotation is symbolized by k_m. The Shubnikov notation and the international notation use the same symbols for screw rotations. The symbols for glide reflections in both notations are listed in Table 3.3.2.1.

If the point-group symbol contains only one generator, the related space group is described completely by the Bravais lattice and a symbol corresponding to that of the point group in which rotations and reflections are replaced by screw rotations or glide reflections, if necessary. If, however, two or more operations generate the point group, it is necessary to have information on the mutual orientations and locations of the corresponding space-group symmetry elements, *i.e.* information on the location components $\boldsymbol{w}_l$. This is described in the following sections.

3.3.2.4. Shubnikov symbols

For the description of the mutual orientation of symmetry elements, the same symbols as for point groups are applied. In space groups, however, the symmetry elements need not intersect. In this case, the orientational symbols · (dot), : (colon), / (slash) are modified to $\odot$, $\vdots$, //. The space-group symbol starts with a description of the lattice defined by the basis **a**, **b**, **c**. For centred cells, the vectors to the centring points are given first. The same letters are used for basis vectors related by symmetry. The relative orientations of the vectors are denoted by the orientational symbols introduced above. The description of the lattice given in parentheses is followed by symbols of the generating elements of the related point group. If necessary, the symbols of the symmetry operations are modified to indicate their glide/screw parts. The first generator is separated from the lattice description by an orientation symbol. If this generator represents a mirror or glide plane, the dot connects the plane with the last two vectors whereas the colon refers only to the last vector. If the generator represents a rotation or a rotoreflection, the colon orients the related axis perpendicular to the plane given by the last two vectors whereas the dot refers only to the last vector. Two generators are separated by the symbols mentioned above to denote their relative orientations and sites. To make this description unique for space groups related to point group $O_h \equiv \tilde{6}/4$ with Bravais lattices *cP* and *cF*, it is necessary to use three generators instead of two: $4/\tilde{6}\cdot m$. For the sake of unifi-

cation, this kind of description is extended to the remaining two space groups having Bravais lattice *cI*.

Example: Shubnikov symbol for the space group with Schoenflies symbol D_{2h}^{26} (*72*)

The Bravais lattice is *oI* (orthorhombic, body-centred). Therefore, the symbol for the lattice basis is

$$\left(\frac{a+b+c}{2}\middle/ c:(a:b)\right),$$

indicating that there is a centring vector $1/2(\mathbf{a}+\mathbf{b}+\mathbf{c})$ relative to the conventional orthorhombic cell. This vector is oblique with respect to the basis vector **c**, which is orthogonal to the perpendicular pair **a** and **b**. The basis vectors have independent lengths and are thus indicated by different letters *a*, *b* and *c* in arbitrary sequence.

To complete the symbol of the space group, we consider the point group D_{2h}. Its Shubnikov symbol is $m:2\cdot m$. Parallel to the (**a**, **b**) plane, there is a glide plane $\widetilde{ab}$ and a mirror plane *m*. The latter is chosen as generator. From the screw axis 2_1 and the rotation axis 2, both parallel to **c**, the latter is chosen as generator. The third generator can be a glide plane *c* perpendicular to **b**. Thus the Shubnikov symbol of D_{2h}^{26} is

$$\left(\frac{a+b+c}{2}\middle/ c:(a:b)\right)\cdot m:2\cdot\tilde{c}.$$

The list of all Shubnikov symbols is given in column 3 of Table 3.3.3.1.

3.3.2.5. International short symbols

The international symbol of a space group consists of two parts, just like the Shubnikov symbol. The first part is a capital letter that describes the type of centring of the conventional cell. It is followed by a modified point-group symbol that refers to the lattice symmetry directions. Centring type and point-group symbol determine the Bravais type of the translation group (*cf.* Section 3.1.1) and thus the point group of the lattice and the appropriate lattice symmetry directions. To derive the short international symbol of a given space group, the short symbol of the related point group must be modified in such a way that not only the rotation parts of the generating operations but also their translation parts can be constructed. This can be done by the following procedure:

(i) The glide/screw parts of generators and indicators are symbolized by applying the symbols for glide planes in Table 3.3.2.1 and the appropriate rules for screw rotations.

(ii) The generators are chosen in such a way that the related symmetry elements do intersect as far as possible. Exceptions may occur for space groups related to the pure rotation point groups 222, 422, 622, 23 and 432. In these cases, the axes of the generators may or may not intersect.

(iii) Subgroups of lattice point groups may have lattice symmetry directions with which no symmetry elements are associated. Such symmetry directions are symbolized by '1'. This symbol can only be omitted if no ambiguity arises, *e.g.* $P4/m11$ is reduced to $P4/m$. $P31m$ and $P3m1$, however, cannot be reduced. The use of the symbol '1' is discussed by Buerger (1967) and Donnay (1969, 1977).

Example

Again consider space group D_{2h}^{26} (72). The space group contains glide planes *c* and *b* perpendicular to the primary set, *c* and *a* normal to the secondary set of symmetry directions and *m* and *n* perpendicular to the tertiary set. To determine the short symbol, one generator must be chosen from each pair. The standardization rules (see the following section) lead to the symbol *Ibam*.

3.3.3. Properties of the international symbols

3.3.3.1. Derivation of the space group from the short symbol

Because the short international symbol contains a set of generators, it is possible to deduce the space group from it. With the same distinction between generators and indicators as for point groups, the modified point-group symbol directly gives the rotation parts $\boldsymbol{W}$ of the generating operations ($\boldsymbol{W}$, $\boldsymbol{w}$).

The modified symbols of the generators determine the glide/screw parts $\boldsymbol{w}_g$ of $\boldsymbol{w}$. To find the location parts $\boldsymbol{w}_l$ of $\boldsymbol{w}$, it is necessary to inspect the product relations of the group. The deduction of the set of complete generating operations can be summarized in the following rules:

(i) The integral translations are included in the set of generators. If the unit cell has centring points, the centring operations are generators.

(ii) The location parts of the generators can be set to zero except for the two cases noted under (iii) and (iv).

(iii) For non-cubic rotation groups with indicators in the symbol, the location part of the first generator can be set to zero. The location part of the second generator is $\boldsymbol{w}_l=\begin{pmatrix}0\\0\\-m/n\end{pmatrix}$; the intersection parameter $-m/n$ is derived from the indicator n_m in the [001] direction [*cf.* example (3) below].

(iv) For cubic rotation groups, the location part of the threefold rotation can be set to zero. For space groups related to the point group 23, the location part of the twofold rotation is $\boldsymbol{w}_l=\begin{pmatrix}-m/n\\0\\0\end{pmatrix}$ derived from the symbol n_m of the twofold operation itself. For space groups related to the point group 432, the location part of the twofold generating rotation is $\boldsymbol{w}_l=\begin{pmatrix}-m/n\\m/n\\m/n\end{pmatrix}$ derived from the indicator n_m in the [001] direction [*cf.* examples (4) and (5) below].

The origin that is selected by these rules is called the '*origin of the symbol*' (Burzlaff & Zimmermann, 1980). It is evident that the reference to the origin of the symbol allows a very short and unique notation of all desirable origins by appending the components of the origin of the symbol $\mathbf{q}=(q_1,q_2,q_3)$ to the short space-group symbol, thus yielding the so-called *expanded* Hermann–Mauguin symbol. The shift of origin can be performed easily, for only the translation parts have to be changed. The components of the transformed translation part can be obtained by [*cf.* Section 1.5.2.3 and equation (1.5.2.13)]

$$\boldsymbol{w}'=\boldsymbol{w}+(\boldsymbol{W}-\boldsymbol{I})\boldsymbol{q}.$$

Applications can be found in Burzlaff & Zimmermann (2002).

Examples: Deduction of the generating operations from the short symbol

Some examples for the use of these rules are now described in detail. It is convenient to describe the symmetry operation

($\boldsymbol{W}$, $\boldsymbol{w}$) by the corresponding coordinate triplets, *i.e.* using the so-called shorthand notation, *cf.* Section 1.2.2. The coordinate triplets can be interpreted as combinations of two constituents: the first one consists of the coordinates of a point in general position after the application of $\boldsymbol{W}$ on x, y, z, while the second corresponds to the translation part $\boldsymbol{w}$ of the symmetry operation. The coordinate triplets of the symmetry operations are tabulated as the *general position* in the space-group tables (in some cases a shift of origin is necessary). If preference is given to full matrix notation, Table 1.2.2.1 may be used. The following examples contain, besides the description of the symmetry operations, references to the numbering of the general positions in the space-group tables of this volume; *cf.* Sections 2.1.3.9 and 2.1.3.11. Centring translations are written after the numbers, if necessary.

(1) $Pccm = D_{2h}^{3}$ (49)

Besides the integral translations, the generators, as given in the symbol, are according to rule (ii):

glide reflection	c_{100}:	$\overline{x}, y, z+\frac{1}{2}$	(8)
glide reflection	c_{010}:	$x, \overline{y}, z+\frac{1}{2}$	(7)
reflection	m_{001}:	$x, y, \overline{z}$	(6).

No shift of origin is necessary. The expanded symbol is $Pccm\langle 000\rangle$.

(2) $Ibam = D_{2h}^{26}$ (72)

According to rule (i), the I centring is an additional generating translation. Thus, the generators are:

I centring:		$x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$	$(1)+(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
glide reflection	b_{100}:	$\overline{x}, y+\frac{1}{2}, z$	(8)
glide reflection	a_{010}:	$x+\frac{1}{2}, \overline{y}, z$	(7)
reflection	m_{001}:	$x, y, \overline{z}$	(6).

To obtain the tabulated general position, a shift of origin by $(-\frac{1}{4},-\frac{1}{4},0)$ is necessary, the expanded symbol is $Ibam\langle -\frac{1}{4}-\frac{1}{4}0\rangle$.

(3) $P4_12_12 = D_4^4$ (92)

Apart from the translations, the generating elements are:

screw rotation 2_1 in	[100]:	$x+\frac{1}{2}, \overline{y}, \overline{z}$	(6)
rotation 2 in	$[1\overline{1}0]$:	$\overline{y}, \overline{x}, \overline{z}+\frac{1}{4}$	(8).

According to rule (iii), the location part of the first generator, referring to the secondary set of symmetry directions, is equal to zero. For the second generator, the screw part is equal to zero. The location part is $\boldsymbol{w}_l = \begin{pmatrix} 0 \\ 0 \\ -\frac{1}{4} \end{pmatrix}$. The expanded symbol $P4_12_12\langle\frac{1}{4}-\frac{1}{4}-\frac{3}{8}\rangle$ gives the tabulated setting.

(4) $P2_13 = T^4$ (198)

According to rule (iv), the generators are

rotation 3 in	[111]:	z, x, y	(5)
screw rotation 2_1 in	[001]:	$\overline{x}+\frac{1}{2}, \overline{y}, z+\frac{1}{2}$	(2).

Following rule (iv), the location part of the threefold axis must be set to zero. The screw part of the twofold axis in [001] is $\begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$, the location part is $\boldsymbol{w}_l = \begin{pmatrix} -\frac{1}{2} \\ 0 \\ 0 \end{pmatrix} \equiv \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}$. No origin shift is necessary. The expanded symbol is $P2_13\langle 000\rangle$.

(5) $P4_132 = O^7$ (213)

Besides the integral translations, the generators given by the symbol are:

rotation 3 in	[111]:	z, x, y	(5)
rotation 2 in	[110]:	$y-\frac{1}{4}, x+\frac{1}{4}, \overline{z}+\frac{1}{4}$	(13).

The screw part of the twofold axis is zero. According to rule (iv), the location part is $\boldsymbol{w}_l = \begin{pmatrix} -\frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix}$. No origin shift is necessary. The expanded symbol is $P4_132\langle 000\rangle$.

3.3.3.2. Derivation of the full symbol from the short symbol

If the geometrical point of view is again considered, it is possible to derive the full international symbol for a space group. This full symbol can be interpreted as consisting of symmetry elements. It can be generated from the short symbol with the aid of products between symmetry operations. It is possible, however, to derive the glide/screw parts of the elements in the full symbol directly from the glide/screw parts of the short symbol.

The product of operations corresponding to non-parallel glide or mirror planes generates a rotation or screw axis parallel to the intersection line. The screw part of the rotation is equal to the sum of the projections of the glide components of the planes on the axis. The angle between the planes determines the rotation part of the axis. For 90°, we obtain a twofold, for 60° a threefold, for 45° a fourfold and for 30° a sixfold axis.

Example: $Pbcn = D_{2h}^{14}$ (60)

The product of b and c generates a screw axis 2_1 in the z direction because the sum of the glide components in the z direction is $\frac{1}{2}$. The product of c and n generates a screw axis 2_1 in the x direction and the product between b and n produces a rotation axis 2 in the y direction because the y components for b and n add up to $1 \equiv 0$ modulo integers.

Thus, the full symbol is

$$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}.$$

In most cases, the full symbol is identical with the short symbol; differences between full and short symbols can only occur for space groups corresponding to lattice point groups (holohedries) and to the point group $m\overline{3}$. In all these cases, the short symbol is extended to the full symbol by adding the symbol for the maximal purely rotational subgroup. A special procedure is in use for monoclinic space groups. To indicate the choice of coordinate axes, the full symbol is treated like an orthorhombic symbol, in which the directions without symmetry are indicated by '1', *even though they do not correspond to lattice symmetry directions in the monoclinic case.*

3.3.3.3. Non-symbolized symmetry elements

Certain symmetry elements are not given explicitly in the full symbol because they can easily be derived. They are:

(i) Rotoinversion axes that are not used to indicate the lattice symmetry directions.

(ii) Rotation axes 2 included in the axes 4, $\overline{4}$ and 6 and rotation axes 3 included in the axes $\overline{3}$, 6 and $\overline{6}$.

(iii) Additional symmetry elements occurring in space groups with centred unit cells, *cf.* Sections 1.4.2.4 and 1.5.4.1. These types of operation can be deduced from the product of the centring translation $(\boldsymbol{I}, \boldsymbol{g})$ with a symmetry operation $(\boldsymbol{W}, \boldsymbol{w})$. The new symmetry operation $(\boldsymbol{W}, \boldsymbol{g}+\boldsymbol{w})$ again has $\boldsymbol{W}$ as rotation part but a different glide/screw part if the component of $\boldsymbol{g}$ parallel to the symmetry element corresponding to $\boldsymbol{W}$ is not a lattice vector; *cf.* Section 1.5.4.1.

Example

Space group $C2/c$ (15) has a twofold axis along **b** with screw part $\boldsymbol{w}_g = \begin{pmatrix}0\\0\\0\end{pmatrix}$. The translational part of the centring operation is $\boldsymbol{g} = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix}$.

An additional axis parallel to **b** thus has a translation part $\boldsymbol{g}+\boldsymbol{w}_g = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix}$. The component $\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}$ indicates a screw axis 2_1 in the b direction, whereas the component $\begin{pmatrix}\frac{1}{2}\\0\\0\end{pmatrix}$ indicates the location of this axis in $\frac{1}{4}, y, 0$. Similarly, it can be shown that glide plane c combined with the centring gives a glide plane n.

In the same way, in rhombohedral and cubic space groups, a rotation axis 3 is accompanied by screw axes 3_1 and 3_2. In space groups with centred unit cells, the location parts of different symmetry elements may coincide. In $I\bar{4}2m$, for example, the mirror plane m contains simultaneously a non-symbolized glide plane n. The same applies to all mirror planes in *Fmmm*.

(iv) Symmetry elements with diagonal orientation always occur with different types of glide/screw parts simultaneously. In space group $P\bar{4}2m$ (111) the translation vector along a can be decomposed as

$$\boldsymbol{w} = \begin{pmatrix}1\\0\\0\end{pmatrix} = \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix} + \begin{pmatrix}\frac{1}{2}\\-\frac{1}{2}\\0\end{pmatrix} = \boldsymbol{w}_g + \boldsymbol{w}_l.$$

The diagonal mirror plane with normal along $[1\bar{1}0]$ passing through the origin is accompanied by a parallel glide plane with glide part $\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix}$ passing through $\frac{1}{4}, -\frac{1}{4}, 0$. The same arguments lead to the occurrence of screw axes 2_1, 3_1 and 3_2 connected with diagonal rotation axes 2 or 3.

(v) For some investigations connected with *klassengleiche* subgroups (for subgroups of space groups, *cf.* Section 1.7.1), it is convenient to introduce an *extended Hermann–Mauguin symbol* that comprises all symmetry elements indicated in (iii) and (iv). The basic concept may be found in papers by Hermann (1929) and in *IT* (1952). These concepts have been applied by Bertaut (1976) and Zimmermann (1976); *cf.* Section 1.5.4.1.

Example

The full symbol of space group *Imma* (74) is

$$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}.$$

The I-centring operation introduces additional rotation axes and glide planes for all three sets of lattice symmetry directions. The extended Hermann–Mauguin symbol is

$$I\frac{2,2_1}{m,n}\frac{2,2_1}{m,n}\frac{2,2_1}{a,b} \quad \text{or} \quad I\begin{matrix}\frac{2_1}{m} & \frac{2_1}{m} & \frac{2_1}{a}\\ \frac{2}{n} & \frac{2}{n} & \frac{2}{b}\end{matrix}.$$

This symbol shows immediately the eight subgroups with a P lattice corresponding to point group *mmm*:

$Pmma \sim Pmmb$, $Pnma \sim Pmnb$, $Pmna \sim Pnmb$ and $Pnna \sim Pnnb$.

3.3.3.4. Standardization rules for short symbols

The symbols of Bravais lattices and glide planes depend on the choice of basis vectors. As shown in the preceding section, additional translation vectors in centred unit cells produce new symmetry operations with the same rotation but different glide/screw parts. Moreover, it was shown that for diagonal orientations symmetry operations may be represented by different symbols. Thus, different short symbols for the same space group can be derived even if the rules for the selection of the generators and indicators are obeyed.

For the unique designation of a space-group type, a standardization of the short symbol is necessary. Rules for standardization were given first by Hermann (1931) and later in a slightly modified form in *IT* (1952).

These rules, which are generally followed in the present tables, are given below. Because of the historical development of the symbols (*cf.* Section 3.3.4), some of the present symbols do not obey the rules, whereas others depending on the crystal class need additional rules for them to be uniquely determined. These exceptions and additions are not explicitly mentioned, but may be discovered from Table 3.3.3.1 in which the short symbols are listed for all space groups. A table for all settings may be found in Section 1.5.4.

Triclinic symbols are unique if the unit cell is primitive. For the standard setting of *monoclinic* space groups, the lattice symmetry direction is labelled b. From the three possible centrings A, I and C, the latter one is favoured. If glide components occur in the plane perpendicular to [010], the glide direction c is preferred. In the space groups corresponding to the *orthorhombic* group $mm2$, the unique direction of the twofold axis is chosen along **c**. Accordingly, the face centring C is employed for centrings perpendicular to the privileged direction. For space groups with possible A or B centring, the first one is preferred. For groups 222 and *mmm*, no privileged symmetry direction exists, so the different possibilities of one-face centring can be reduced to C centring by change of the setting. The choices of unit cell and centring type are fixed by the conventional basis in systems with higher symmetry.

When more than one kind of symmetry elements exist in one representative direction, in most cases the choice for the space-group symbol is made in order of decreasing priority: for reflections and glide reflections m, a, b, c, n, d; for proper rotations and screw rotations 6, 6_1, 6_2, 6_3, 6_4, 6_5; 4, 4_1, 4_2, 4_3; 3, 3_1, 3_2; 2, 2_1 [*cf. IT* (1952), p. 55, and Section 1.4.1].

(*continued on page* 789)

Table 3.3.3.1
Standard space-group symbols

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
1	C_1^1	$(a/b/c)\cdot 1$	$P1$	$P1$	$P1$	$P1$	
2	C_i^1	$(a/b/c)\cdot \bar{2}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$(a/b/c)\cdot \bar{1}$ (Sh–K)
3	C_2^1	$(b:(c/a)):2$	$P2$	$P2$	$P2$	$P121$	
		$(c:(a/b)):2$				$P112$	
4	C_2^2	$(b:(c/a)):2_1$	$P2_1$	$P2_1$	$P2_1$	$P12_11$	
		$(c:(a/b)):2_1$				$P112_1$	
5	C_2^3	$\left(\frac{a+b}{2}\middle/ b:(c/a)\right):2$	$C2$	$C2$	$C2$	$C121$	$B2$, $B112$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\middle/ c:(b/a)\right):2$				$A112$	$\left(\frac{a+c}{2}\middle/ c:(a/b)\right):2$ (Sh–K)
6	C_2^1	$(b:(c/a))\cdot m$	Pm	Pm	Pm	$P1m1$	
		$(c:(a/b))\cdot m$				$P11m$	
7	C_s^2	$(b:(c/a))\cdot \tilde{c}$	Pc	Pc	Pc	$P1c1$	Pb, $P11b$ (*IT*, 1952)
		$(c:(b/a))\cdot \tilde{a}$				$P11a$	$(c:(a/b))\cdot \tilde{b}$ (Sh–K)
8	C_s^3	$\left(\frac{a+b}{2}\middle/ b:(c/a)\right)\cdot m$	Cm	Cm	Cm	$C1m1$	Bm, $B11m$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\middle/ c:(b/a)\right)\cdot m$				$A11m$	$\left(\frac{a+c}{2}\middle/ c:(a/b)\right)\cdot m$ (Sh–K)
9	C_s^4	$\left(\frac{a+b}{2}\middle/ b:(c/a)\right)\cdot \tilde{c}$	Cc	Cc	Cc	$C1c1$	Bb, $B11b$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\middle/ c:(b/a)\right)\cdot \tilde{a}$				$A11a$	$\left(\frac{a+c}{2}\middle/ c:(a/b)\right)\cdot \tilde{b}$ (Sh–K)
10	C_{2h}^1	$(b:(c/a))\cdot m:2$	$P2/m$	$P2/m$	$P2/m$	$P1\ 2/m1$	
		$(c:(a/b))\cdot m:2$				$P11\ 2/m$	
11	C_{2h}^2	$(b:(c/a))\cdot m:2_1$	$P2_1/m$	$P2_1/m$	$P2_1/m$	$P1\ 2_1/m\ 1$	
		$(c:(a/b))\cdot m:2_1$				$P11\ 2_1/m$	
12	C_{2h}^3	$\left(\frac{a+b}{2}\middle/ b:(c/a)\right)\cdot m:2$	$C2/m$	$C2/m$	$C2/m$	$C1\ 2/m\ 1$	$B2/m$, $B11\ 2/m$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\middle/ c:(b/a)\right)\cdot m:2$				$A11\ 2/m$	$\left(\frac{a+c}{2}\middle/ c:(a/b)\right)\cdot m:2$ (Sh–K)
13	C_{2h}^4	$(b:(c/a))\cdot \tilde{c}:2$	$P2/c$	$P2/c$	$P2/c$	$P1\ 2/c\ 1$	$P2/b$, $P11\ 2/b$ (*IT*, 1952)
		$(c:(a/b))\cdot \tilde{a}:2$				$P11\ 2/a$	$(c:(a/b))\cdot \tilde{b}:2$ (Sh–K)
14	C_{2h}^5	$(b:(c/a))\cdot \tilde{c}:2_1$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P1\ 2_1/c\ 1$	$P2_1/b$, $P112_1/b$ (*IT*, 1952)
		$(c:(a/b))\cdot \tilde{a}:2_1$				$P11\ 2_1/a$	$(c:(a/b))\cdot b:2_1$ (Sh–K)
15	C_{2h}^6	$\left(\frac{a+b}{2}\middle/ b:(c/a)\right)\cdot \tilde{c}:2$	$C2/c$	$C2/c$	$C2/c$	$C1\ 2/c\ 1$	$B2/b$, $B11\ 2/b$ (*IT*, 1952)
		$\left(\frac{b+c}{2}\middle/ c:(b/a)\right)\cdot \tilde{a}:2$				$A11\ 2a$	$\left(\frac{a+c}{2}\middle/ c:(a/b)\right)\cdot \tilde{b}:2$ (Sh–K)
16	D_2^1	$(c:(a:b)):2:2$	$P222$	$P222$	$P222$	$P222$	
17	D_2^2	$(c:(a:b)):2_1:2$	$P222_1$	$P222_1$	$P222_1$	$P222_1$	
18	D_2^3	$(c:(a:b)):2\odot 2_1$	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P2_12_12$	
19	D_2^4	$(c:(a:b)):2_1\odot 2_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	
20	D_2^5	$\left(\frac{a+b}{2}:c:(a:b)\right):2_1:2$	$C222_1$	$C222_1$	$C222_1$	$C222_1$	
21	D_2^6	$\left(\frac{a+b}{2}:c:(a:b)\right):2:2$	$C222$	$C222$	$C222$	$C222$	
22	D_2^7	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}:c:(a:b)\right):2:2$	$F222$	$F222$	$F222$	$F222$	
23	D_2^8	$\left(\frac{a+b+c}{2}\middle/ c:(a:b)\right):2:2$	$I222$	$I222$	$I222$	$I222$	
24	D_2^9	$\left(\frac{a+b+c}{2}\middle/ c:(a:b)\right):2:2_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	$I2_12_12_1$	
25	C_{2v}^1	$(c:(a:b)):m\cdot 2$	Pmm	$Pmm2$	$Pmm2$	$Pmm2$	
26	C_{2v}^2	$(c:(a:b)):\tilde{c}\cdot 2_1$	Pmc	$Pmc2_1$	$Pmc2_1$	$Pmc2_1$	
27	C_{2v}^3	$(c:(a:b)):\tilde{c}\cdot 2$	Pcc	$Pcc2$	$Pcc2$	$Pcc2$	

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
28	C_{2v}^{4}	$(c:(a:b)):\tilde{a}\cdot 2$	*Pma*	*Pma*2	*Pma*2	*Pma*2	
29	C_{2v}^{5}	$(c:(a:b)):\tilde{a}\cdot 2_1$	*Pca*	*Pca*2_1	*Pca*2_1	*Pca*2_1	
30	C_{2v}^{6}	$(c:(a:b)):\tilde{c}\odot 2$	*Pnc*	*Pnc*2	*Pnc*2	*Pnc*2	$(c:(a:b)):\widetilde{ac}\cdot 2$ (Sh–K)
31	C_{2v}^{7}	$(c:(a:b)):\widetilde{ac}\cdot 2_1$	*Pmn*	*Pmn*2_1	*Pmn*2_1	*Pmn*2_1	
32	C_{2v}^{8}	$(c:(a:b)):\tilde{a}\odot 2$	*Pba*	*Pba*2	*Pba*2	*Pba*2	
33	C_{2v}^{9}	$(c:(a:b)):\tilde{a}\odot 2_1$	*Pna*	*Pna*2_1	*Pna*2_1	*Pna*2_1	
34	C_{2v}^{10}	$(c:(a:b)):\widetilde{ac}\odot 2$	*Pnn*	*Pnn*2	*Pnn*2	*Pnn*2	
35	C_{2v}^{11}	$\left(\frac{a+b}{2}:c:(a:b)\right):m\cdot 2$	*Cmm*	*Cmm*2	*Cmm*2	*Cmm*2	
36	C_{2v}^{12}	$\left(\frac{a+b}{2}:c:(a:b)\right):\tilde{c}\cdot 2_1$	*Cmc*	*Cmc*2_1	*Cmc*2_1	*Cmc*2_1	
37	C_{2v}^{13}	$\left(\frac{a+b}{2}:c:(a:b)\right):\tilde{c}\cdot 2$	*Ccc*	*Ccc*2	*Ccc*2	*Ccc*2	
38	C_{2v}^{14}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):m\cdot 2$	*Amm*	*Amm*2	*Amm*2	*Amm*2	
39	C_{2v}^{15}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):m\cdot 2_1$	*Abm*	*Abm*2	*Aem*2	*Aem*2	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):\tilde{c}\cdot 2$ (Sh−K) Use former symbol *Abm*2 for generation
40	C_{2v}^{16}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2$	*Ama*	*Ama*2	*Ama*2	*Ama*2	
41	C_{2v}^{17}	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2_1$	*Aba*	*Aba*2	*Aea*2	*Aea*2	$\left(\frac{b+c}{2}\Big/c:(a:b)\right):\widetilde{ac}\cdot 2$ (Sh−K) Use former symbol *Aba*2 for generation
42	C_{2v}^{18}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:c:(a:b)\right):m\cdot 2$	*Fmm*	*Fmm*2	*Fmm*2	*Fmm*2	
43	C_{2v}^{19}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}:\tilde{c}:(a:b)\right):\frac{1}{2}\widetilde{ac}\odot 2$	*Fdd*	*Fdd*2	*Fdd*2	*Fdd*2	
44	C_{2v}^{20}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):m\cdot 2$	*Imm*	*Imm*2	*Imm*2	*Imm*2	
45	C_{2v}^{21}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):\tilde{c}\cdot 2$	*Iba*	*Iba*2	*Iba*2	*Iba*2	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2_1$ (Sh–K)
46	C_{2v}^{22}	$\left(\frac{a+b+c}{2}\Big/c:(a:b)\right):\tilde{a}\cdot 2$	*Ima*	*Ima*2	*Ima*2	*Ima*2	
47	D_{2h}^{1}	$(c:(a:b))\cdot m:2\cdot m$	*Pmmm*	*P*2/*m* 2/*m* 2/*m*	*Pmmm*	*P*2/*m* 2/*m* 2/*m*	
48	D_{2h}^{2}	$(c:(a:b))\cdot\widetilde{ab}:2\odot\widetilde{ac}$	*Pnnn*	*P*2/*n* 2/*n* 2/*n*	*Pnnn*	*P*2/*n* 2/*n* 2/*n*	
49	D_{2h}^{3}	$(c:(a:b))\cdot m:2\cdot\tilde{c}$	*Pccm*	*P*2/*c* 2/*c* 2/*m*	*Pccm*	*P*2/*c* 2/*c* 2/*m*	
50	D_{2h}^{4}	$(c:(a:b))\cdot\widetilde{ab}:2\odot\tilde{a}$	*Pban*	*P*2/*b* 2/*a* 2/*n*	*Pban*	*P*2/*b* 2/*a* 2/*n*	
51	D_{2h}^{5}	$(c:(a:b))\cdot\tilde{a}:2\cdot m$	*Pmma*	*P*2_1/*m* 2/*m* 2/*a*	*Pmma*	*P*2_1/*m* 2/*m* 2/*a*	
52	D_{2h}^{6}	$(c:(a:b))\cdot\tilde{a}:2\odot\widetilde{ac}$	*Pnna*	*P*2/*n* 2_1/*n* 2/*a*	*Pnna*	*P*2/*n* 2_1/*n* 2/*a*	
53	D_{2h}^{7}	$(c:(a:b))\cdot\tilde{a}:2_1\cdot\widetilde{ac}$	*Pmna*	*P*2/*m* 2/*n* 2_1/*a*	*Pmna*	*P*2/*m* 2/*n* 2_1/*a*	
54	D_{2h}^{8}	$(c:(a:b))\cdot\tilde{a}:2\cdot\tilde{c}$	*Pcca*	*P*2_1/*c* 2/*c* 2/*a*	*Pcca*	*P*2_1/*c* 2/*c* 2/*a*	
55	D_{2h}^{9}	$(c:(a:b))\cdot m:2\odot\tilde{a}$	*Pbam*	*P*2_1/*b* 2_1/*a* 2/*m*	*Pbam*	*P*2_1/*b* 2_1/*a* 2/*m*	
56	D_{2h}^{10}	$(c:(a:b))\cdot\widetilde{ab}:2\cdot\tilde{c}$	*Pccn*	*P*2_1/*c* 2_1/*c* 2/*n*	*Pccn*	*P*2_1/*c* 2_1/*c* 2/*n*	
57	D_{2h}^{11}	$(c:(a:b))\cdot m:2_1\odot\tilde{c}$	*Pbcm*	*P*2/*b* 2_1/*c* 2_1/*m*	*Pbcm*	*P*2/*b* 2_1/*c* 2_1/*m*	
58	D_{2h}^{12}	$(c:(a:b))\cdot m:2\odot\widetilde{ac}$	*Pnnm*	*P*2_1/*n* 2_1/*n* 2/*m*	*Pnnm*	*P*2_1/*n* 2_1/*n* 2/*m*	
59	D_{2h}^{13}	$(c:(a:b))\cdot\widetilde{ab}:2\cdot m$	*Pmmn*	*P*2_1/*m* 2_1/*m* 2/*n*	*Pmmn*	*P*2_1/*m* 2_1/*m* 2/*n*	
60	D_{2h}^{14}	$(c:(a:b))\cdot\widetilde{ab}:2_1\odot\tilde{c}$	*Pbcn*	*P*2_1/*b* 2/*c* 2_1/*n*	*Pbcn*	*P*2_1/*b* 2/*c* 2_1/*n*	
61	D_{2h}^{15}	$(c:(a:b))\cdot\tilde{a}:2_1\odot\tilde{c}$	*Pbca*	*P*2_1/*b* 2_1/*c* 2_1/*a*	*Pbca*	*P*2_1/*b* 2_1/*c* 2_1/*a*	
62	D_{2h}^{16}	$(c:(a:b))\cdot\tilde{a}:2_1\odot m$	*Pnma*	*P*2_1/*n* 2_1/*m* 2_1/*a*	*Pnma*	*P*2_1/*n* 2_1/*m* 2_1/*a*	
63	D_{2h}^{17}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot m:2_1\cdot\tilde{c}$	*Cmcm*	*C*2/*m* 2/*c* 2_1/*m*	*Cmcm*	*C*2/*m* 2/*c* 2_1/*m*	
64	D_{2h}^{18}	$\left(\frac{a+b}{2}:c:(a:b)\right)\cdot\tilde{a}:2_1\cdot\tilde{c}$	*Cmca*	*C*2/*m* 2/*c* 2_1/*a*	*Cmce*	*C*2/*m* 2/*c* 2_1/*e*	Use former symbol *Cmca* for generation

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
65	D_{2h}^{19}	$\left(\frac{a+b}{2}{:}c{:}(a{:}b)\right)\cdot m{:}2\cdot m$	*Cmmm*	*C*2/*m* 2/*m* 2/*m*	*Cmmm*	*C*2/*m* 2/*m* 2/*m*	
66	D_{2h}^{20}	$\left(\frac{a+b}{2}{:}c{:}(a{:}b)\right)\cdot m{:}2\cdot \tilde{c}$	*Cccm*	*C*2/*c* 2/*c* 2/*m*	*Cccm*	*C*2/*c* 2/*c* 2/*m*	
67	D_{2h}^{21}	$\left(\frac{a+b}{2}{:}c{:}(a{:}b)\right)\cdot \tilde{a}{:}2\cdot m$	*Cmma*	*C*2/*m* 2/*m* 2/*a*	*Cmme*	*C*2/*m* 2/*m* 2/*e*	Use former symbol *Cmma* for generation
68	D_{2h}^{22}	$\left(\frac{a+b}{2}{:}c{:}(a{:}b)\right)\cdot \tilde{a}{:}2\cdot \tilde{c}$	*Ccca*	*C*2/*c* 2/*c* 2/*a*	*Ccce*	*C*2/*c* 2/*c* 2/*e*	Use former symbol *Ccca* for generation
69	D_{2h}^{23}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}c{:}(a{:}b)\right)\cdot m{:}2\cdot m$	*Fmmm*	*F*2/*m* 2/*m* 2/*m*	*Fmmm*	*F*2/*m* 2/*m* 2/*m*	
70	D_{2h}^{24}	$\left(\frac{a+c}{2}\Big/\frac{b+c}{2}\Big/\frac{a+b}{2}{:}c{:}(a{:}b)\right)\cdot \frac{1}{2}\tilde{a}\tilde{b}{:}2\odot\frac{1}{2}\tilde{a}\tilde{c}$	*Fddd*	*F*2/*d* 2/*d* 2/*d*	*Fddd*	*F*2/*d* 2/*d* 2/*d*	
71	D_{2h}^{25}	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}b)\right)\cdot m{:}2\cdot m$	*Immm*	*I*2/*m* 2/*m* 2/*m*	*Immm*	*I*2/*m* 2/*m* 2/*m*	
72	D_{2h}^{26}	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}b)\right)\cdot m{:}2\cdot \tilde{c}$	*Ibam*	*I*2/*b* 2/*a* 2/*m*	*Ibam*	*I*2/*b* 2/*a* 2/*m*	
73	D_{2h}^{27}	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}b)\right)\cdot \tilde{a}{:}2\cdot \tilde{c}$	*Ibca*	$I2_1/b\ 2_1/c\ 2_1/a$	*Ibca*	$I2_1/b\ 2_1/c\ 2_1/a$	*I*2/*b* 2/*c* 2/*a* (*IT*, 1952)
74	D_{2h}^{28}	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}b)\right)\cdot \tilde{a}{:}2\cdot m$	*Imma*	$I2_1/m\ 2_1/m\ 2_1/a$	*Imma*	$I2_1/m\ 2_1/m\ 2_1/a$	*I*2/*m* 2/*m* 2/*a* (*IT*, 1952)
75	C_4^1	$(c{:}(a{:}a)){:}4$	*P*4	*P*4	*P*4	*P*4	
76	C_4^2	$(c{:}(a{:}a)){:}4_1$	$P4_1$	$P4_1$	$P4_1$	$P4_1$	
77	C_4^3	$(c{:}(a{:}a)){:}4_2$	$P4_2$	$P4_2$	$P4_2$	$P4_2$	
78	C_4^4	$(c{:}(a{:}a)){:}4_3$	$P4_3$	$P4_3$	$P4_3$	$P4_3$	
79	C_4^5	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}a)\right){:}4$	*I*4	*I*4	*I*4	*I*4	
80	C_4^6	$\left(\frac{a-b-c}{2}\Big/c{:}(a{:}a)\right){:}4_1$	$I4_1$	$I4_1$	$I4_1$	$I4_1$	
81	S_4^1	$(c{:}(a{:}a)){:}\tilde{4}$	$P\bar{4}$	$P\bar{4}$	$P\bar{4}$	$P\bar{4}$	
82	S_4^2	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}a)\right){:}\tilde{4}$	$I\bar{4}$	$I\bar{4}$	$I\bar{4}$	$I\bar{4}$	
83	C_{4h}^1	$(c{:}(a{:}a))\cdot m{:}4$	*P*4/*m*	*P*4/*m*	*P*4/*m*	*P*4/*m*	
84	C_{4h}^2	$(c{:}(a{:}a))\cdot m{:}4_2$	$P4_2/m$	$P4_2/m$	$P4_2/m$	$P4_2/m$	
85	C_{4h}^3	$(c{:}(a{:}a))\cdot \tilde{a}\tilde{b}{:}4$	*P*4/*n*	*P*4/*n*	*P*4/*n*	*P*4/*n*	
86	C_{4h}^4	$(c{:}(a{:}a))\cdot \tilde{a}\tilde{b}{:}4_2$	$P4_2/n$	$P4_2/n$	$P4_2/n$	$P4_2/n$	
87	C_{4h}^5	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}a)\right)\cdot m{:}4$	*I*4/*m*	*I*4/*m*	*I*4/*m*	*I*4/*m*	
88	C_{4h}^6	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}a)\right)\cdot \tilde{a}{:}4_1$	$I4_1/a$	$I4_1/a$	$I4_1/a$	$I4_1/a$	
89	D_4^1	(*c*:(*a*:*a*)):4:2	*P*42	*P*422	*P*422	*P*422	
90	D_4^2	$(c{:}(a{:}a)){:}4\odot 2_1$	$P42_1$	$P42_12$	$P42_12$	$P42_12$	
91	D_4^3	$(c{:}(a{:}a)){:}4_1{:}2$	$P4_12$	$P4_122$	$P4_122$	$P4_122$	
92	D_4^4	$(c{:}(a{:}a)){:}4_1\odot 2_1$	$P4_12_1$	$P4_12_12$	$P4_12_12$	$P4_12_12$	
93	D_4^5	$(c{:}(a{:}a)){:}4_2{:}2$	$P4_22$	$P4_222$	$P4_222$	$P4_222$	
94	D_4^6	$(c{:}(a{:}a)){:}4_2\odot 2_1$	$P4_22_1$	$P4_22_12$	$P4_22_12$	$P4_22_12$	
95	D_4^7	$(c{:}(a{:}a)){:}4_3{:}2$	$P4_32$	$P4_322$	$P4_322$	$P4_322$	
96	D_4^8	$(c{:}(a{:}a)){:}4_3\odot 2_1$	$P4_32_1$	$P4_32_12$	$P4_32_12$	$P4_32_12$	
97	D_4^9	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}a)\right){:}4{:}2$	*I*42	*I*422	*I*422	*I*422	
98	D_4^{10}	$\left(\frac{a+b+c}{2}\Big/c{:}(a{:}a)\right){:}4_1{:}2$	$I4_12$	$I4_122$	$I4_122$	$I4_122$	
99	C_{4v}^1	$(c{:}(a{:}a)){:}4\cdot m$	*P*4*mm*	*P*4*mm*	*P*4*mm*	*P*4*mm*	
100	C_{4v}^2	$(c{:}(a{:}a)){:}4\odot \tilde{a}$	*P*4*bm*	*P*4*bm*	*P*4*bm*	*P*4*bm*	
101	C_{4v}^3	$(c{:}(a{:}a)){:}4_2\cdot \tilde{c}$	*P*4*cm*	$P4_2cm$	$P4_2cm$	$P4_2cm$	
102	C_{4v}^4	$(c{:}(a{:}a)){:}4_2\odot \tilde{a}\tilde{c}$	*P*4*nm*	$P4_2nm$	$P4_2nm$	$P4_2nm$	

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
103	C_{4v}^{5}	$(c\!:\!(a\!:\!a))\!:\!4\cdot\tilde{c}$	*P*4*cc*	*P*4*cc*	*P*4*cc*	*P*4*cc*	
104	C_{4v}^{6}	$(c\!:\!(a\!:\!a))\!:\!4\odot\widetilde{ac}$	*P*4*nc*	*P*4*nc*	*P*4*nc*	*P*4*nc*	
105	C_{4v}^{7}	$(c\!:\!(a\!:\!a))\!:\!4_2\cdot m$	*P*4*mc*	*P*4$_2$*mc*	*P*4$_2$*mc*	*P*4$_2$*mc*	
106	C_{4v}^{8}	$(c\!:\!(a\!:\!a))\!:\!4_2\odot\tilde{a}$	*P*4*bc*	*P*4$_2$*bc*	*P*4$_2$*bc*	*P*4$_2$*bc*	
107	C_{4v}^{9}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!4\cdot m$	*I*4*mm*	*I*4*mm*	*I*4*mm*	*I*4*mm*	
108	C_{4v}^{10}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!4\cdot\tilde{c}$	*I*4*cm*	*I*4*cm*	*I*4*cm*	*I*4*cm*	
109	C_{4v}^{11}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!4_1\odot m$	*I*4*md*	*I*4$_1$*md*	*I*4$_1$*md*	*I*4$_1$*md*	
110	C_{4v}^{12}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!4_1\odot\tilde{c}$	*I*4*cd*	*I*4$_1$*cd*	*I*4$_1$*cd*	*I*4$_1$*cd*	$\left(\underset{\text{(Sh–K)}}{\frac{a+b+c}{2}}\middle/c\!:\!a\!:\!a\right)\!:\!4_1\cdot\tilde{a}$
111	D_{2d}^{1}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\!:\!2$	*P*$\bar{4}$2*m*	*P*$\bar{4}$2*m*	*P*$\bar{4}$2*m*	*P*$\bar{4}$2*m*	
112	D_{2d}^{2}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\,\tilde{:}\,2$	*P*$\bar{4}$2*c*	*P*$\bar{4}$2*c*	*P*$\bar{4}$2*c*	*P*$\bar{4}$2*c*	
113	D_{2d}^{3}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\cdot\widetilde{ab}$	*P*$\bar{4}$2$_1$*m*	*P*$\bar{4}$2$_1$*m*	*P*$\bar{4}$2$_1$*m*	*P*$\bar{4}$2$_1$*m*	
114	D_{2d}^{4}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\cdot\widetilde{abc}$	*P*$\bar{4}$2$_1$*c*	*P*$\bar{4}$2$_1$*c*	*P*$\bar{4}$2$_1$*c*	*P*$\bar{4}$2$_1$*c*	
115	D_{2d}^{5}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\cdot m$	*C*$\bar{4}$2*m*	*C*$\bar{4}$2*m*	*P*$\bar{4}$*m*2	*P*$\bar{4}$*m*2	
116	D_{2d}^{6}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\cdot\tilde{c}$	*C*$\bar{4}$2*c*	*C*$\bar{4}$2*c*	*P*$\bar{4}$*c*2	*P*$\bar{4}$*c*2	
117	D_{2d}^{7}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\odot\tilde{a}$	*C*$\bar{4}$2*b*	*C*$\bar{4}$2*b*	*P*$\bar{4}$*b*2	*P*$\bar{4}$*b*2	
118	D_{2d}^{8}	$(c\!:\!(a\!:\!a))\!:\!\tilde{\bar{4}}\cdot\widetilde{ac}$	*C*$\bar{4}$2*n*	*C*$\bar{4}$2*n*	*P*$\bar{4}$*n*2	*P*$\bar{4}$*n*2	
119	D_{2d}^{9}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!\tilde{\bar{4}}\cdot m$	*F*$\bar{4}$2*m*	*F*$\bar{4}$2*m*	*I*$\bar{4}$*m*2	*I*$\bar{4}$*m*2	
120	D_{2d}^{10}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!\tilde{\bar{4}}\cdot\tilde{c}$	*F*$\bar{4}$2*c*	*F*$\bar{4}$2*c*	*I*$\bar{4}$*c*2	*I*$\bar{4}$*c*2	
121	D_{2d}^{11}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!\tilde{\bar{4}}\!:\!2$	*I*$\bar{4}$2*m*	*I*$\bar{4}$2*m*	*I*$\bar{4}$2*m*	*I*$\bar{4}$2*m*	
122	D_{2d}^{12}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\!:\!\tilde{4}\odot\frac{1}{2}\widetilde{abc}$	*I*$\bar{4}$2*d*	*I*$\bar{4}$2*d*	*I*$\bar{4}$2*d*	*I*$\bar{4}$2*d*	
123	D_{4h}^{1}	$(c\!:\!(a\!:\!a))\cdot m\!:\!4\cdot m$	*P*4/*mmm*	*P*4/*m* 2/*m* 2/*m*	*P*4/*mmm*	*P*4/*m* 2/*m* 2/*m*	
124	D_{4h}^{2}	$(c\!:\!(a\!:\!a))\cdot m\!:\!4\cdot\tilde{c}$	*P*4/*mcc*	*P*4/*m* 2/*c* 2/*c*	*P*4/*mcc*	*P*4/*m* 2/*c* 2/*c*	
125	D_{4h}^{3}	$(c\!:\!(a\!:\!a))\cdot\widetilde{ab}\!:\!4\odot\tilde{a}$	*P*4/*nbm*	*P*4/*n* 2/*b* 2/*m*	*P*4/*nbm*	*P*4/*n* 2/*b* 2/*m*	$(c\!:\!a\!:\!a)\cdot\widetilde{ab}\!:\!4\odot\tilde{b}$ (Sh–K)
126	D_{4h}^{4}	$(c\!:\!(a\!:\!a))\cdot\widetilde{ab}\!:\!4\odot\widetilde{ac}$	*P*4/*nnc*	*P*4/*n* 2/*n* 2/*c*	*P*4/*nnc*	*P*4/*n* 2/*n* 2/*c*	
127	D_{4h}^{5}	$(c\!:\!(a\!:\!a))\cdot m\!:\!4\odot\tilde{a}$	*P*4/*mbm*	*P*4/*m* 2$_1$/*b* 2/*m*	*P*4/*mbm*	*P*4/*m* 2$_1$/*b* 2/*m*	$(c\!:\!a\!:\!a)\cdot m\!:\!4\odot\tilde{b}$ (Sh–K)
128	D_{4h}^{6}	$(c\!:\!(a\!:\!a))\cdot m\!:\!4\odot\widetilde{ac}$	*P*4/*mnc*	*P*4/*m* 2$_1$/*n* 2/*c*	*P*4/*mnc*	*P*4/*m* 2$_1$/*n* 2/*c*	
129	D_{4h}^{7}	$(c\!:\!(a\!:\!a))\cdot\widetilde{ab}\!:\!4\cdot m$	*P*4/*nmm*	*P*4/*n* 2$_1$/*m* 2/*m*	*P*4/*nmm*	*P*4/*n* 2$_1$/*m* 2/*m*	
130	D_{4h}^{8}	$(c\!:\!(a\!:\!a)\cdot\widetilde{ab}\!:\!4\cdot\tilde{c}$	*P*4/*ncc*	*P*4/*n* 2/*c* 2/*c*	*P*4/*ncc*	*P*4/*n* 2/*c* 2/*c*	
131	D_{4h}^{9}	$(c\!:\!(a\!:\!a))\cdot m\!:\!4_2\cdot m$	*P*4/*mmc*	*P*4$_2$/*m* 2/*m* 2/*c*	*P*4$_2$/*mmc*	*P*4$_2$/*m* 2/*m* 2/*c*	
132	D_{4h}^{10}	$(c\!:\!(a\!:\!a))\cdot m\!:\!4_2\cdot\tilde{c}$	*P*4/*mcm*	*P*4$_2$/*m* 2/*c* 2/*m*	*P*4$_2$/*mcm*	*P*4$_2$/*m* 2/*c* 2/*m*	
133	D_{4h}^{11}	$(c\!:\!(a\!:\!a))\cdot\widetilde{ab}\!:\!4_2\odot\tilde{a}$	*P*4/*nbc*	*P*4$_2$/*n* 2/*b* 2/*c*	*P*4$_2$/*nbc*	*P*4$_2$/*n* 2/*b* 2/*c*	$(c\!:\!a\!:\!a)\cdot\widetilde{ab}\!:\!4_2\odot\tilde{b}$ (Sh–K)
134	D_{4h}^{12}	$(c\!:\!(a\!:\!a))\cdot\widetilde{ab}\!:\!4_2\odot\widetilde{ac}$	*P*4/*nnm*	*P*4$_2$/*n* 2/*n* 2/*m*	*P*4$_2$/*nnm*	*P*4$_2$/*n* 2/*n* 2/*m*	
135	D_{4h}^{13}	$(c\!:\!(a\!:\!a))\cdot n\!:\!4_2\odot\tilde{a}$	*P*4/*mbc*	*P*4$_2$/*m* 2$_1$/*b* 2/*c*	*P*4$_2$/*mbc*	*P*4$_2$/*m* 2$_1$/*b* 2/*c*	$(c\!:\!a\!:\!a)\cdot m\!:\!4_2\odot\tilde{b}$ (Sh–K)
136	D_{4h}^{14}	$(c\!:\!(a\!:\!a))\cdot m\!:\!4_2\odot\widetilde{ac}$	*P*4/*mnm*	*P*4$_2$/*m* 2$_1$/*n* 2/*m*	*P*4$_2$/*mnm*	*P*4$_2$/*m* 2$_1$/*n* 2/*m*	
137	D_{4h}^{15}	$(c\!:\!(a\!:\!a))\cdot\widetilde{ab}\!:\!4_2\cdot m$	*P*4/*nmc*	*P*4$_2$/*n* 2$_1$/*m* 2/*c*	*P*4$_2$/*nmc*	*P*4$_2$/*n* 2$_1$/*m* 2/*c*	
138	D_{4h}^{16}	$(c\!:\!(a\!:\!a))\cdot ab\!:\!4_2\cdot\tilde{c}$	*P*4/*ncm*	*P*4$_2$/*n* 2$_1$/*c* 2/*m*	*P*4$_2$/*ncm*	*P*4$_2$/*n* 2$_1$/*c* 2/*m*	
139	D_{4h}^{17}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\cdot m\!:\!4\cdot m$	*I*4/*mmm*	*I*4/*m* 2/*m* 2/*m*	*I*4/*mmm*	*I*4/*m* 2/*m* 2/*m*	
140	D_{4h}^{18}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\cdot m\!:\!4\cdot\tilde{c}$	*I*4/*mcm*	*I*4/*m* 2/*c* 2/*m*	*I*4/*mcm*	*I*4/*m* 2/*c* 2/*m*	
141	D_{4h}^{19}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\cdot\tilde{a}\!:\!4_1\odot m$	*I*4/*amd*	*I*4$_1$/*a* 2/*m* 2/*d*	*I*4$_1$/*amd*	*I*4$_1$/*a* 2/*m* 2/*d*	
142	D_{4h}^{20}	$\left(\frac{a+b+c}{2}\middle/c\!:\!(a\!:\!a)\right)\cdot\tilde{a}\!:\!4_1\odot\tilde{c}$	*I*4/*acd*	*I*4$_1$/*a* 2/*c* 2/*d*	*I*4$_1$/*acd*	*I*4$_1$/*a* 2/*c* 2/*d*	
143	C_{3}^{1}	$(c\!:\!(a/a))\!:\!3$	*C*3	*C*3	*P*3	*P*3	
144	C_{3}^{2}	$(c\!:\!(a/a))\!:\!3_1$	*C*3$_1$	*C*3$_1$	*P*3$_1$	*P*3$_1$	
145	C_{3}^{3}	$(c\!:\!(a/a))\!:\!3_2$	*C*3$_2$	*C*3$_2$	*P*3$_2$	*P*3$_2$	

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
146	C_3^4	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c{:}(a/a)\right)$: 3	$R3$	$R3$	$R3$	$R3$	Hexagonal setting (Sh–K)
		$(a/a/a)/3$					Rhombohedral setting (Sh–K)
147	C_{3i}^1	$(c{:}(a/a)){:}\tilde{6}$	$C\bar{3}$	$C\bar{3}$	$P\bar{3}$	$P\bar{3}$	
148	C_{3i}^2	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c{:}(a/a)\right)$: $\tilde{6}$	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6}$					Rhombohedral setting (Sh–K)
149	D_3^1	$(c{:}(a/a)){:}2{:}3$	$H32$	$H321$	$P312$	$P312$	
150	D_3^2	$(c{:}(a/a)){:}2{:}3$	$C32$	$C321$	$P321$	$P321$	
151	D_3^3	$(c{:}(a/a)){:}2{:}3_1$	$H3_12$	$H3_121$	$P3_112$	$P3_112$	
152	D_3^4	$(c{:}(a/a)){:}2{:}3_1$	$C3_12$	$C3_121$	$P3_121$	$P3_121$	
153	D_3^5	$(c{:}(a/a)){:}2{:}3_2$	$H3_22$	$H3_221$	$P3_212$	$P3_212$	
154	D_3^6	$(c{:}(a/a)){:}2{:}3_2$	$C3_22$	$C3_221$	$P3_221$	$P3_221$	
155	D_3^7	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c{:}(a/a)\right)$ ·2:3	$R32$	$R32$	$R32$	$R32$	Hexagonal setting (Sh–K)
		$(a/a/a)/3{:}2$					Rhombohedral setting (Sh–K)
156	C_{3v}^1	$(c{:}(a/a)){:}m{:}3$	$C3m$	$C3m1$	$P3m1$	$P3m1$	
157	C_{3v}^2	$(a{:}c{:}a){:}m{:}3$	$H3m$	$H3m1$	$P31m$	$P31m$	$(c{:}(a/a)) \cdot m \cdot 3$ (Sh–K) with special comment
158	C_{3v}^3	$(c{:}(a/a)){:}\tilde{c}{:}3$	$C3c$	$C3c1$	$P3c1$	$P3c1$	
159	C_{3v}^4	$(a{:}c{:}a){:}\tilde{c}{:}3$	$H3c$	$H3c1$	$P31c$	$P31c$	$(c{:}(a/a)) \cdot \tilde{c} \cdot 3$ (Sh–K) with special comment
160	C_{3v}^5	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c{:}(a/a)\right)$ $\cdot m \cdot 3$	$R3m$	$R3m$	$R3m$	$R3m$	Hexagonal setting (Sh–K)
		$(a/a/a)/3 \cdot m$					Rhombohedral setting (Sh–K)
161	C_{3v}^6	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c{:}(a/a)\right)$ $\cdot \tilde{c} \cdot 3$	$R3c$	$R3c$	$R3c$	$R3c$	Hexagonal setting (Sh–K)
		$(a/a/a)/3 \cdot \widetilde{abc}$					Rhombohedral setting (Sh–K)
162	D_{3d}^1	$(a{:}c{:}a) \cdot m \cdot \tilde{6}$	$H\bar{3}m$	$H\bar{3}\ 2/m\ 1$	$P\bar{3}1m$	$P\bar{3}1\ 2/m$	$(c{:}(a/a)) \cdot m \cdot \tilde{6}$ (Sh–K) with special comment
163	D_{3d}^2	$(a{:}c{:}a) \cdot \tilde{c} \cdot \tilde{6}$	$H\bar{3}c$	$H\bar{3}\ 2/c\ 1$	$P\bar{3}1c$	$P\bar{3}1\ 2/c$	$(c{:}(a/a) \cdot \tilde{c} \cdot \tilde{6}$ (Sh–K) with special comment
164	D_{3d}^3	$(c{:}(a/a)){:}m \cdot \tilde{6}$	$C\bar{3}m$	$C\bar{3}\ 2/m\ 1$	$P\bar{3}m1$	$P\bar{3}\ 2/m\ 1$	
165	D_{3d}^4	$(c{:}(a/a)){:}\tilde{c} \cdot \tilde{6}$	$C\bar{3}c$	$C\bar{3}\ 2/c\ 1$	$P\bar{3}c1$	$P\bar{3}\ 2/c\ 1$	
166	D_{3d}^5	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c{:}(a/a)\right)$: $m \cdot \tilde{6}$	$R\bar{3}m$	$R\bar{3}\ 2/m$	$R\bar{3}m$	$R\bar{3}\ 2/m$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6} \cdot m$					Rhombohedral setting (Sh–K)
167	D_{3d}^6	$\left(\frac{2a+b+c}{3}\Big/\frac{a+2b+2c}{3}\Big/c{:}(a/a)\right)$: $\tilde{c} \cdot \tilde{6}$	$R\bar{3}c$	$R\bar{3}\ 2/c$	$R\bar{3}c$	$R\bar{3}\ 2/c$	Hexagonal setting (Sh–K)
		$(a/a/a)/\tilde{6} \cdot \widetilde{abc}$					Rhombohedral setting (Sh–K)
168	C_6^1	$(c{:}(a/a)){:}6$	$C6$	$C6$	$P6$	$P6$	
169	C_6^2	$(c{:}(a/a)){:}6_1$	$C6_1$	$C6_1$	$P6_1$	$P6_1$	
170	C_6^3	$(c{:}(a/a)){:}6_5$	$C6_5$	$C6_5$	$P6_5$	$P6_5$	
171	C_6^4	$(c{:}(a/a)){:}6_2$	$C6_2$	$C6_2$	$P6_2$	$P6_2$	
172	C_6^5	$(c{:}(a/a)){:}6_4$	$C6_4$	$C6_4$	$P6_4$	$P6_4$	
173	C_6^6	$(c{:}(a/a)){:}6_3$	$C6_3$	$C6_3$	$P6_3$	$P6_3$	
174	C_{3h}^1	$(c{:}(a/a)){:}3{:}m$	$C\bar{6}$	$C\bar{6}$	$P\bar{6}$	$P\bar{6}$	
175	C_{6h}^1	$(c{:}(a/a)) \cdot m{:}6$	$C6/m$	$C6/m$	$P6/m$	$P6/m$	
176	C_{6h}^2	$(c{:}(a/a)) \cdot m{:}6_3$	$C6_3/m$	$C6_3/m$	$P6_3/m$	$P6_3/m$	

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
177	D_6^1	$(c\!:\!(a/a))\cdot 2\!:\!6$	*C*62	*C*622	*P*622	*P*622	
178	D_6^2	$(c\!:\!(a/a))\cdot 2\!:\!6_1$	$C6_12$	$C6_122$	$P6_122$	$P6_122$	
179	D_6^3	$(c\!:\!(a/a))\cdot 2\!:\!6_5$	$C6_52$	$C6_522$	$P6_522$	$P6_522$	
180	D_6^4	$(c\!:\!(a/a))\cdot 2\!:\!6_2$	$C6_22$	$C6_222$	$P6_222$	$P6_222$	
181	D_6^5	$(c\!:\!(a/a))\cdot 2\!:\!6_4$	$C6_42$	$C6_422$	$P6_422$	$P6_422$	
182	D_6^6	$(c\!:\!(a/a))\cdot 2\!:\!6_3$	$C6_32$	$C6_322$	$P6_322$	$P6_322$	
183	C_{6v}^1	$(c\!:\!(a/a))\!:\!m\cdot 6$	*C*6*mm*	*C*6*mm*	*P*6*mm*	*P*6*mm*	
184	C_{6v}^2	$(c\!:\!(a/a))\!:\!\tilde{c}\cdot 6$	*C*6*cc*	*C*6*cc*	*P*6*cc*	*P*6*cc*	
185	C_{6v}^3	$(c\!:\!(a/a))\!:\!\tilde{c}\cdot 6_3$	*C*6*cm*	$C6_3cm$	$P6_3cm$	$P6_3cm$	
186	C_{6v}^4	$(c\!:\!(a/a))\!:\!m\cdot 6_3$	*C*6*mc*	$C6_3mc$	$P6_3mc$	$P6_3mc$	
187	D_{3h}^1	$(c\!:\!(a/a))\!:\!m\cdot 3\!:\!m$	$C\bar{6}m2$	$C\bar{6}m2$	$P\bar{6}m2$	$P\bar{6}m2$	
188	D_{3h}^2	$(c\!:\!(a/a))\!:\!\tilde{c}\cdot 3\!:\!m$	$C\bar{6}c2$	$C\bar{6}c2$	$P\bar{6}c2$	$P\bar{6}c2$	
189	D_{3h}^3	$(c\!:\!(a/a))\cdot m\!:\!3\cdot m$	$H\bar{6}m2$	$H\bar{6}m2$	$P\bar{6}2m$	$P\bar{6}2m$	
190	D_{3h}^4	$(c\!:\!(a/a))\cdot m\!:\!3\cdot \tilde{c}$	$H\bar{6}c2$	$H\bar{6}c2$	$P\bar{6}2c$	$P\bar{6}2c$	
191	D_{6h}^1	$(c\!:\!(a/a))\cdot m\!:\!6\cdot m$	*C*6/*mmm*	*C*6/*m* 2/*m* 2/*m*	*P*6/*mmm*	*P*6/*m* 2/*m* 2/*m*	
192	D_{6h}^2	$(c\!:\!(a/a))\cdot m\!:\!6\cdot \tilde{c}$	*C*6/*mcc*	*C*6/*m* 2/*c* 2/*c*	*P*6/*mcc*	*P*6/*m* 2/*c* 2/*c*	
193	D_{6h}^3	$(c\!:\!(a/a))\cdot m\!:\!6_3\cdot \tilde{c}$	*C*6/*mcm*	$C6_3/m$ 2/*c* 2/*m*	$P6_3/mcm$	$P6_3/m$ 2/*c* 2/*m*	
194	D_{6h}^4	$(c\!:\!(a/a))\cdot m\!:\!6_3\cdot m$	*C*6/*mmc*	$C6_3/m$ 2/*m* 2/*c*	$P6_3/mmc$	$P6_3/m$ 2/*m* 2/*c*	
195	T^1	$(a\!:\!(a/a))\!:\!2/3$	*P*23	*P*23	*P*23	*P*23	
196	T^2	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}\!:\!a\!:\!(a\!:\!a)\right)\!:\!2/3$	*F*23	*F*23	*F*23	*F*23	
197	T^3	$\left(\frac{a+b+c}{2}\middle/a\!:\!(a\!:\!a)\right)\!:\!2/3$	*I*23	*I*23	*I*23	*I*23	
198	T^4	$(a\!:\!(a\!:\!a))\!:\!2_1//3$	$P2_13$	$P2_13$	$P2_13$	$P2_13$	
199	T^5	$\left(\frac{a+b+c}{2}\middle/a\!:\!(a\!:\!a)\right)\!:\!2_1//3$	$I2_13$	$I2_13$	$I2_13$	$I2_13$	
200	T_h^1	$(a\!:\!(a\!:\!a))\cdot m/\tilde{6}$	*Pm*3	$P2/m\ \bar{3}$	$Pm\bar{3}$	$P2/m\ \bar{3}$	*Pm*3 (*IT*, 1952)
201	T_h^2	$(a\!:\!(a\!:\!a))\cdot \tilde{a}\tilde{b}/\tilde{6}$	*Pn*3	$P2/n\ \bar{3}$	$Pn\bar{3}$	$P2/n\ \bar{3}$	*Pn*3 (*IT*, 1952)
202	T_h^3	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}\!:\!a\!:\!(a\!:\!a)\right)\cdot m/\tilde{6}$	*Fm*3	$F2/m\ \bar{3}$	$Fm\bar{3}$	$F2/m\ \bar{3}$	*Fm*3 (*IT*, 1952)
203	T_h^4	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}\!:\!a\!:\!(a\!:\!a)\right)\cdot\frac{1}{2}ab/\tilde{6}$	*Fd*3	$F2/d\ \bar{3}$	$Fd\bar{3}$	$F2/d\ \bar{3}$	*Fd*3 (*IT*, 1952)
204	T_h^5	$\left(\frac{a+b+c}{2}\middle/a\!:\!(a\!:\!a)\right)\cdot m/\tilde{6}$	*Im*3	$I2/m\ \bar{3}$	$Im\bar{3}$	$I2/m\ \bar{3}$	*Im*3 (*IT*, 1952)
205	T_h^6	$(a\!:\!(a\!:\!a))\cdot \tilde{a}/\tilde{6}$	*Pa*3	$P2_1/a\ \bar{3}$	$Pa\bar{3}$	$P2_1/a\ \bar{3}$	*Pa*3 (*IT*, 1952)
206	T_h^7	$\left(\frac{a+b+c}{2}\middle/a\!:\!(a\!:\!a)\right)\cdot \tilde{a}/\tilde{6}$	*Ia*3	$I2_1/a\ \bar{3}$	$Ia\bar{3}$	$I2_1/a\ \bar{3}$	*Ia*3 (*IT*, 1952)
207	O^1	$(a\!:\!(a\!:\!a))\!:\!4/3$	*P*43	*P*432	*P*432	*P*432	
208	O^2	$(a\!:\!(a\!:\!a))\!:\!4_2//3$	$P4_23$	$P4_232$	$P4_232$	$P4_232$	
209	O^3	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}\!:\!a\!:\!(a\!:\!a)\right)\!:\!4/3$	*F*43	*F*432	*F*432	*F*432	
210	O^4	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}\!:\!a\!:\!(a\!:\!a)\right)\!:\!4_1//3$	$F4_13$	$F4_132$	$F4_132$	$F4_132$	
211	O^5	$\left(\frac{a+b+c}{2}\middle/a\!:\!(a\!:\!a)\right)\!:\!4/3$	*I*43	*I*432	*I*432	*I*432	
212	O^6	$(a\!:\!(a\!:\!a))\!:\!4_3//3$	$P4_33$	$P4_332$	$P4_332$	$P4_332$	
213	O^7	$(a\!:\!(a\!:\!a))\!:\!4_1//3$	$P4_13$	$P4_132$	$P4_132$	$P4_132$	
214	O^8	$\left(\frac{a+b+c}{2}\middle/a\!:\!(a\!:\!a)\right)\!:\!4_1//3$	$I4_13$	$I4_132$	$I4_132$	$I4_132$	

Table 3.3.3.1 (continued)

No.	Schoenflies symbol	Shubnikov symbol	Symbols of *International Tables*				Comments†
			1935 Edition		Present Edition		
			Short	Full	Short	Full	
215	T_d^1	$(a:(a:a)):\tilde{4}/3$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	$P\bar{4}3m$	
216	T_d^2	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}:a:(a:a)\right):\tilde{4}/3$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	$F\bar{4}3m$	
217	T_d^3	$\left(\frac{a+b+c}{2}\middle/a:(a:a)\right):\tilde{4}/3$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	$I\bar{4}3m$	
218	T_d^4	$(a:(a:a)):\tilde{4}//3$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	$P\bar{4}3n$	
219	T_d^5	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}:a:(a:a)\right):\tilde{4}//3$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	$F\bar{4}3c$	
220	T_d^6	$\left(\frac{a+b+c}{2}\middle/a:(a:a)\right):\tilde{4}//3$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	$I\bar{4}3d$	
221	O_h^1	$(a:(a:a)):4/\tilde{6}\cdot m$	$Pm3m$	$P4/m\ \bar{3}\ 2/m$	$Pm\bar{3}m$	$P4/m\ \bar{3}\ 2/m$	$Pm3m$ (*IT*, 1952)
222	O_h^2	$(a:(a:a)):4/\tilde{6}\cdot\widetilde{abc}$	$Pn3n$	$P4/n\ \bar{3}\ 2/n$	$Pn\bar{3}n$	$P4/n\ \bar{3}\ 2/n$	$Pn3n$ (*IT*, 1952)
223	O_h^3	$(a:(a:a)):4_2//\tilde{6}\cdot\widetilde{abc}$	$Pm3n$	$P4_2/m\ \bar{3}\ 2/n$	$Pm\bar{3}n$	$P4_2/m\ \bar{3}\ 2/n$	$Pm3n$ (*IT*, 1952)
224	O_h^4	$(a:(a:a)):4_2//\tilde{6}\cdot m$	$Pn3m$	$P4_2/n\ \bar{3}\ 2/m$	$Pn\bar{3}m$	$P4_2/n\ \bar{3}\ 2/m$	$Pn3m$ (*IT* ,1952)
225	O_h^5	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot m$	$Fm3m$	$F4/m\ \bar{3}\ 2/m$	$Fm\bar{3}m$	$F4/m\ \bar{3}\ 2/m$	$Fm3m$ (*IT*, 1952)
226	O_h^6	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}:a:(a:a)\right):4/\tilde{6}\cdot\tilde{c}$	$Fm3c$	$F4/m\ \bar{3}\ 2/c$	$Fm\bar{3}c$	$F4/m\ \bar{3}\ 2/c$	$Fm3c$ (*IT*, 1952)
227	O_h^7	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}:a(a:a)\right):4_1//\tilde{6}\cdot m$	$Fd3m$	$F4_1/d\ \bar{3}\ 2/m$	$Fd\bar{3}m$	$F4_1/d\ \bar{3}\ 2/m$	$Fd3m$ (*IT*, 1952)
228	O_h^8	$\left(\frac{a+c}{2}\middle/\frac{b+c}{2}\middle/\frac{a+b}{2}:a:(a:a)\right):4_1//\tilde{6}\cdot\tilde{c}$	$Fd3c$	$F4_1/d\ \bar{3}\ 2/c$	$Fd\bar{3}c$	$F4_1/d\ \bar{3}\ 2/c$	$Fd3c$ (*IT*, 1952)
229	O_h^9	$\left(\frac{a+b+c}{2}\middle/a:(a:a)\right):4/\tilde{6}\cdot m$	$Im3m$	$I4/m\ \bar{3}\ 2/m$	$Im\bar{3}m$	$I4/m\ \bar{3}\ 2/m$	$Im3m$ (*IT*, 1952)
230	O_h^{10}	$\left(\frac{a+b+c}{2}\middle/a:(a:a)\right):4_1//\tilde{6}\cdot\frac{1}{2}\widetilde{abc}$	$Ia3d$	$I4_1/a\ \bar{3}\ 2/d$	$Ia\bar{3}d$	$I4_1/a\ \bar{3}\ 2/d$	$Ia3d$ (*IT*, 1952)

† Abbreviations used in the column *Comments*: *IT*, 1952: *International Tables for X-ray Crystallography*, Vol. I (1952); Sh–K; Shubnikov & Koptsik (1972). Note that this table contains only one notation for the *b*-unique setting and one notation for the *c*-unique setting in the monoclinic case, always referring to cell choice 1 of the space-group tables.

3.3.3.5. Systematic absences

Hermann (1928*a*) emphasized that the short symbols permit the derivation of systematic absences of X-ray reflections caused by the glide/screw parts of the symmetry operations. If $\boldsymbol{h} = (hkl)$ describes the X-ray reflection and $(\boldsymbol{W}, \boldsymbol{w})$ is the matrix representation of a symmetry operation, the matrix can be expanded as follows:

$$(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{W}, \boldsymbol{w}_g + \mathbf{w}_l) = (\boldsymbol{W}, \begin{pmatrix} w_{g,1} \\ w_{g,2} \\ w_{g,3} \end{pmatrix} + \boldsymbol{w}_l).$$

The absence of a reflection is governed by the relation (i) $\boldsymbol{h} \cdot \boldsymbol{W} = \boldsymbol{h}$ and the scalar product (ii) $\boldsymbol{h} \cdot \boldsymbol{w}_g = hw_{g,1} + kw_{g,2} + lw_{g,3}$. A reflection $\boldsymbol{h}$ is absent if condition (i) holds and the scalar product (ii) is not an integer. The calculation must be made for all generators and indicators of the short symbol. Systematic absences, introduced by the further symmetry operations generated, are obtained by the combination of the extinction rules derived for the generators and indicators.

Example: Space group $D_4^{10} = I4_122$ (98)

The generators of the space group are the integral translations and the centring translation $x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$, the rotation 2 in direction [100]: $x, \overline{y}, \overline{z}$ and the rotation 2 in direction $[1\overline{1}0]$: $\overline{y}, \overline{x}, \overline{z} - \frac{1}{4}$. The combination of the two generators gives the operation corresponding to the indicator, namely $\overline{y}, x, z + \frac{1}{4}$, which represents a fourfold screw rotation in the direction [001].

The integral translations imply no restriction because the scalar product is always an integer. For the centring, condition (i) with $\boldsymbol{W} = \boldsymbol{I}$ holds for all reflections (integral condition), but the scalar product (ii) is an integer only for $h + k + l = 2n$. Thus, reflections *hkl* with $h + k + l \neq 2n$ are absent. The screw rotation 4 has the screw part $\boldsymbol{w}_g = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix}$. Only 00*l* reflections

obey condition (i) (serial extinction). An integral value for the scalar product (ii) requires $l = 4n$. The twofold axes in the directions [100] and [1$\bar{1}$0] do not imply further absences because $\mathbf{w}_g = \mathbf{o}$.

Detailed discussion of the theoretical background of conditions for possible general reflections and their derivation is given in Chapter 1.6.

3.3.3.6. Generalized symmetry

The international symbols can be suitably modified to describe generalized symmetry, *e.g.* colour groups, which occur when the symmetry operations are combined with changes of physical properties. For the description of antisymmetry (or 'black–white' symmetry), the symbols of the Bravais lattices are supplemented by additional letters for centrings accompanied by a change in colour. For symmetry operations that are not translations, a prime is added to the usual symbol if a change of colour takes place. A complete description of the symbols and a detailed list of references are given by Koptsik (1966). The Shubnikov symbols have not been extended to colour symmetry.

An introduction to the structure, properties and symbols of magnetic subperiodic and magnetic space groups is given in Chapter 3.6.

3.3.4. Changes introduced in space-group symbols since 1935

Before the appearance of the first edition of *International Tables* in 1935, different notations for space groups were in use. A summary and comparative tables may be found in the introduction to that edition. The international notation was proposed by Hermann (1928*a*,*b*) and Mauguin (1931), who used the concept of lattice symmetry directions (see Section 3.3.1) and gave preference to reflections or glide reflections as generators. Considerable changes to the original Hermann–Mauguin short symbols were made in *IT* (1952).

The most important change refers to the symmetry directions. In the original Hermann–Mauguin symbols [*IT* (1935)], the distribution of symmetry elements is prescribed by the point-group symbol in the traditional setting, for example $\bar{4}2m$ (not $\bar{4}m2$) but $\bar{6}m2$ (not $\bar{6}2m$). This procedure sometimes implies the use of a larger unit cell than would be necessary. In *IT* (1952) and in the present series, however, the lattice symmetry directions always refer to the conventional cell (*cf.* Chapter 3.1) of the Bravais lattice. The results of this change are (*a*) different symbols for centring types and (*b*) different sequences of the symbols referring to the point group. These differences occur only in some space groups that have a tetragonal or hexagonal lattice.

Thus, the two different space groups D^1_{2d} and D^5_{2d} were symbolized by $P\bar{4}2m$ and $C\bar{4}2m$ in *IT* (1935) because in both cases the twofold axis had to be connected with the secondary set of symmetry directions. The new international symbols are $P\bar{4}2m$ and $P\bar{4}m2$; since in the point group $4/m\ 2/m\ 2/m$ of the Bravais lattice the secondary and tertiary set cannot be distinguished, the twofold axis in the subgroups $\bar{4}2m$ and $\bar{4}m2$ may occur in either the secondary or the tertiary set. Accordingly, the *C*-centred cell of $D^5_{2d} - C\bar{4}2m$, used in *IT* (1935), was transformed to a primitive one with the twofold axis along the tertiary set, resulting in the symbol $P\bar{4}m2$.

The same considerations hold for $\bar{6}m2$ and $\bar{6}2m$ and for space groups with a hexagonal lattice belonging to the point groups 32, $3m$ and $\bar{3}m$, which can be oriented in two ways with respect to the lattice.

For example, the point group $3m$ has two sets of symmetry directions. If the basis vector **a** is normal to the mirror plane *m*, two hexagonal cells with different centrings are possible:

(i) the hexagonal primitive cell, always described by *C* in *IT* (1935), leads to $C3m = C^1_{3v}$;

(ii) the hexagonal *H*-centred cell, with centring points in $\frac{2}{3}, \frac{1}{3}, 0$ and $\frac{1}{3}, \frac{2}{3}, 0$, leads to $H3m = C^2_{3v}$ (*cf.* Chapter 3.1).

The latter can be transformed to a primitive cell in which the mirror plane is normal to the representative of the tertiary set of the hexagonal lattice. In *IT* (1952) and the present editions, the primitive hexagonal cell is described by *P*. Thus, the above space groups receive the symbols $P3m1 = C^1_{3v}$ and $P31m = C^2_{3v}$.

Further changes are:

(i) In *IT* (1952), symbols for space groups related to the point groups 422, 622 and 432 contain the twofold axis of the tertiary set. The advantage is that these groups can be generated by operations of the secondary and tertiary set. The symbol of the indicator is provided with the appropriate index to identify the screw part, thus fixing the intersection parameter.

(ii) Some standard settings are changed in the monoclinic system. In *IT* (1935), only one setting (*b* unique, one cell choice) was tabulated for the monoclinic space groups. In *IT* (1952), two choices were offered, *b* and *c* unique, each with one cell choice. In the present edition, the two choices (*b* and *c* unique) are retained but for each one three different cells are available. The standard short symbol, however, is that of *IT* (1935) (*b*-unique setting).

(iii) In the short symbols of centrosymmetric space groups in the cubic system, $\bar{3}$ is written instead of 3, *e.g.* $Pm\bar{3}$ instead of $Pm3$ [as in *IT* (1935) and *IT* (1952)].

(iv) Beginning with the fourth edition of this volume (1995), the following five orthorhombic space-group symbols have been modified by introducing the new glide-plane symbol *e*, according to a Nomenclature Report of the IUCr (de Wolff *et al.*, 1992).

Space group No.	39	41	64	67	68
Former symbol:	*Abm*2	*Aba*2	*Cmca*	*Cmma*	*Ccca*
New symbol:	*Aem*2	*Aea*2	*Cmce*	*Cmme*	*Ccce*

The new symbol is indicated in the headline of these space groups. Further details are given in Section 2.1.2.

Difficulties arising from these changes are avoided by selecting the lexicographically first one of the two possible glide parts for the generating operation.

Example: $Aea2 \sim Aba2 = C^{17}_{2v}$ (41)

The generators are

A centring:	$x, y + \frac{1}{2}, z + \frac{1}{2}$	$(1) + (0, \frac{1}{2}, \frac{1}{2})$
glide reflection b_{100}:	$\bar{x}, y + \frac{1}{2}, z$	(4)
or glide reflection c_{100}:	$\bar{x}, y, z + \frac{1}{2}$	$(4) + (0, \frac{1}{2}, \frac{1}{2})$
The first possibility is selected.		
glide reflection a_{010}:	$x + \frac{1}{2}, \bar{y}, z$	(3).

A shift of origin by $(-\frac{1}{4}, -\frac{1}{2}, 0)$ is necessary.

The 1935 symbols and all the changes adopted in the present edition of *International Tables* can be seen in Table 3.3.3.1. Differences in the symbols between *IT* (1952) and the present edition may be found in the last column of this table; *cf.* also Section 2.1.3.4.

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3.4. Lattice complexes

W. Fischer and E. Koch

3.4.1. The concept of lattice complexes and limiting complexes

3.4.1.1. Introduction

The term *lattice complex* (*Gitterkomplex*) was originally coined by P. Niggli (1919), but he used the term in an ambiguous manner. Later, Hermann (1935) modified and specified the concept of lattice complexes. The rigorous definition used in this chapter was proposed later still by Fischer & Koch (1974*a*) [*cf.* also Koch & Fischer (1978*a*)]. An alternative definition was given by Zimmermann & Burzlaff (1974) at around the same time.

In crystal structures belonging to different structure types and showing different space-group symmetries, some of the atoms may have the same relative locations (*e.g.* Cl in CsCl and F in CaF_2). The concept of *lattice complexes* can be used to reveal relationships between such crystal structures even if their space groups belong to different types.

The terms 'point configuration' (Fischer & Koch, 1974*a*) and 'crystallographic orbit' (Matsumoto & Wondratschek, 1979) have frequently been used as synonyms for sets of points in three-dimensional space $\mathbb{E}^3$ that are equivalent with respect to a space group $\mathcal{G}$. Such sets of points may be classified in two different ways: (1) according to the concept of lattice complexes (German: *Gitterkomplexe*) and of limiting complexes, which goes back to Hermann (1935) and has been defined more strictly by Fischer & Koch (1974*a*); (2) according to the concept of types of crystallographic orbits and of non-characteristic orbits introduced by Wondratschek (1976). As the two approaches[1] are strongly related but not identical, the classes originating from the two concepts will be compared and the differences worked out.

Both terms, 'point configuration' and 'crystallographic orbit', have been used with two slightly different meanings: (1) for sets of points that are equivalent with respect to a given space group, *i.e.* in the mathematical sense of 'orbit'; (2) for such sets of points, but detached from their generating space groups. The second meaning is referred to, for example, if one speaks only of a primitive cubic point lattice. As within both concepts both meanings are required, one has to distinguish between them. In the following, therefore, the term 'crystallographic orbit' is restricted to the first meaning and the term 'point configuration' is restricted to the second meaning.

3.4.1.2. Crystallographic orbits, Wyckoff positions, Wyckoff sets and types of Wyckoff set

In mathematics, an orbit is a very general group-theoretical term describing any set of objects that are mapped onto each other by the action of a group (*cf.* Section 1.1.7). In fact, orbits are always present in crystallography where equivalence classes are defined by means of a group action (*e.g.* a space-group type is the orbit of a space group in the set of all space groups under the action of the affine group). In the present context, however, the term (crystallographic) orbit will be used in a much more restricted sense, as proposed by Wondratschek (1976):

From any point of $\mathbb{E}^3$, the symmetry operations of a given space group $\mathcal{G}$ generate an infinite set of symmetry-equivalent points, called a *crystallographic orbit with respect to* $\mathcal{G}$ or, for short, a *crystallographic orbit* (*cf.* Section 1.4.4). The space group $\mathcal{G}$ is called the *generating space group* of the orbit.

Each point of a crystallographic orbit defines uniquely a largest finite subgroup of $\mathcal{G}$, which maps that point onto itself, its *site-symmetry group* (*cf.* Section 1.4.4). Site-symmetry groups that belong to different points out of the same crystallographic orbit are conjugate subgroups of $\mathcal{G}$.

Example

The points $x, 0, 0$ and $-x+\frac{1}{2}, 0, \frac{1}{2}$; $-x, 0, 0$ and $x+\frac{1}{2}, 0, \frac{1}{2}$ form an orbit of a given space group *Pmna* together with the infinitely many other points that can be generated from the first four by the translations of *Pmna*. The site-symmetry group 2.. of each such point consists of the identity operation 1 and of a twofold rotation. The position of the twofold axis can easily be read from the corresponding coordinate triplet. The site-symmetry groups of the first two points are $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$, respectively. They can be mapped onto another by conjugation *e.g.* with the glide reflection $a\ x, y, \frac{1}{4}$ of *Pmna*. This glide reflection also interchanges the two twofold axes as can easily be learned by inspecting the space-group diagram.

The crystallographic orbits of a given space group $\mathcal{G}$ subdivide the set of all points of $\mathbb{E}^3$ into equivalence classes. It is also possible, however, to define equivalence of orbits on the set of all crystallographic orbits of $\mathcal{G}$:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same Wyckoff position (*cf.* Section 1.4.4) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of $\mathcal{G}$.[2]

Example

The points $0.2, 0, 0$ and $0.1, 0, 0.5$ belong to different orbits of a given space group *Pmna*. Their site-symmetry groups $\{1; 2\ x, 0, 0\}$ and $\{1; 2\ x, 0, \frac{1}{2}\}$ are conjugate subgroups of *Pmna* (*cf.* the previous example). Therefore, the two orbits belong to the same Wyckoff position of *Pmna*, namely to 4*e*.

The following definition results in a coarser classification of crystallographic orbits:

Two crystallographic orbits of a space group $\mathcal{G}$ belong to the same *Wyckoff set* (German: *Konfigurationslage*, *cf.* Fischer & Koch, 1974*a*) if and only if the site-symmetry groups of any two points stemming from the first and the second orbit are conjugate subgroups of the affine normalizer of $\mathcal{G}$ (*cf.* Section 1.4.4.3).[3]

[1] The following articles are also related to these topics: Engel (1983); Engel *et al.* (1984); Fischer *et al.* (1973); Fischer & Koch (1978, 1983); Koch (1974); Koch & Fischer (1975, 1978*a*, 1985); Steinmann (1984); Wondratschek (1980).

[2] Instead of conjugation by symmetry operations of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used inner automorphisms of $\mathcal{G}$.

[3] Instead of conjugation by elements of the affine normalizer of $\mathcal{G}$, Fischer & Koch (1974*a*) and Koch & Fischer (1975) used automorphisms of $\mathcal{G}$.

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Accordingly, all orbits of a certain Wyckoff position belong to the same Wyckoff set. The assignment of orbits to Wyckoff sets, therefore, also defines an equivalence relation on the Wyckoff positions of a space group. The Wyckoff sets of the space groups were first tabulated by Koch & Fischer (1975).

Example

In space group *Pmna*, the site-symmetry groups of the points 0.2, 0, 0 and 0.2, 0.5, 0 are {1; 2 x, 0, 0} and {1; 2 $x, \frac{1}{2}, 0$}. There is no symmetry operation from *Pmna* that maps these site-symmetry groups onto another by conjugation and hence the two corresponding orbits do not belong to the same Wyckoff position of *Pmna*. The Euclidian (and affine) normalizer of *Pmna* is a space group of type *Pmmm* with half the lattice parameters compared with those of *Pmna* (*cf.* Chapter 3.5). It contains *e.g.* the twofold rotation 2 $x, \frac{1}{4}, 0$ that maps by conjugation the two site-symmetry groups onto another and also the two axes in the space-group diagram. Therefore, the two orbits belong to the same Wyckoff set even though they belong to the different Wyckoff positions 4*e* and 4*f*.

In analogy to the transition from a single space group to its type, it seems desirable to transfer also the terms 'Wyckoff position' and 'Wyckoff set' to the whole space-group type. For Wyckoff positions, however, such a generalization is not possible: two space groups of the same type can be mapped onto each other by infinitely many isomorphisms or affine mappings. Each isomorphism results in a unique relation between the Wyckoff positions of the two groups, but different isomorphisms may give rise to different relations so that the Wyckoff positions of the same Wyckoff set change their roles.

Such ambiguities, however, cannot occur for Wyckoff sets, because all Wyckoff sets of a certain space group differ in their group-theoretical relations to that group. Therefore, Wyckoff sets may be classified as follows:

Two Wyckoff sets stemming from space groups of the same type belong to the same *type of Wyckoff set* if and only if they are related by an isomorphism (affine mapping) of the two space groups (German: *Klasse von Konfigurationslagen*, *cf.* Fischer & Koch, 1974*a*; Koch & Fischer, 1975). The 219 types of space group in $\mathbb{E}^3$ give rise to 1128 types of Wyckoff set.

Example

Take, in a particular space group of type *P*4/*mmm*, the Wyckoff position 4*l* x, 0, 0. The points of each corresponding orbit form squares that replace the points of the tetragonal primitive point lattice of Wyckoff position 1*a*. For all conceivable orbits of 4*l*, the squares have the same orientation, but their edges differ in their lengths. Congruent arrangements of squares but shifted by $\frac{1}{2}\mathbf{c}$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ or by $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$ give the orbits of the Wyckoff positions 4*m*, 4*n* and 4*o*, respectively, in the same space group. The four Wyckoff positions 4*l* to 4*o*, all with site symmetry *m*2*m*., make up a Wyckoff set (*cf.* Table 3.4.3.3). They are mapped onto each other, for example, by the translations $\frac{1}{2}\mathbf{c}$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, which belong to the Euclidean (and affine) normalizer of the group. If one space group of type *P*4/*mmm* is mapped onto another space group of the same type, the Wyckoff set 4*l* to 4*o* as a whole is transformed to 4*l* to 4*o*. The individual Wyckoff positions may be interchanged, however, because of the different possible choices for the origin in each individual space group of type *P*4/*mmm*. All the Wyckoff sets 4*l* to 4*o* stemming from all different space groups of type *P*4/*mmm* constitute together a type of Wyckoff set.

3.4.1.3. Point configurations and lattice complexes, reference symbols

For the comparison of crystal structures belonging to different types, another kind of equivalence relationship between crystallographic orbits may be useful:

One may consider the set of points belonging to a certain orbit without paying attention to the generating space group of the orbit. Such a bare set of points is called a *point configuration*. Two crystallographic orbits are called *configuration equivalent* if their point configurations are identical.

This definition uniquely assigns orbits to point configurations, but not *vice versa*.

Example

Let us consider a certain space group of type $Pm\bar{3}m$ with lattice vectors **a**, **b**, **c** together with two of its non-maximal subgroups, namely $Fm\bar{3}$ with index 4 and *P*432 with index 16, both with lattice vectors 2**a**, 2**b**, 2**c**. The orbit of $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ belongs to Wyckoff position 1*b* of $Pm\bar{3}m$ (site symmetry $m\bar{3}m$), and the corresponding set of points, its point configuration, forms a primitive cubic point lattice. As both subgroups have doubled unit-cell edges, the point $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ turns to $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. The respective orbits belong to Wyckoff position 8*c* of $Fm\bar{3}$ (site symmetry 23.) and to 8*g* of *P*432 (site symmetry .3.), and both correspond to the original point configuration. Therefore, the three orbits $Pm\bar{3}m$ 1*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, $Fm\bar{3}$ 8*c* $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ and *P*432 8*g* x, x, x with $x = \frac{1}{4}$ are configuration equivalent (together with several other orbits from certain other subgroups of $Pm\bar{3}m$). They all give rise to one and the same point configuration, a specific primitive cubic lattice of points. The generating space group, however, cannot be identified just by looking at the point configuration.

The *eigensymmetry* of a point configuration is the most comprehensive space group that maps this point configuration onto itself. Accordingly, exactly one crystallographic orbit out of each class of configuration-equivalent orbits stands out because its generating space group coincides with the eigensymmetry of its point configuration. In the case of the example above, this specific orbit is $Pm\bar{3}m$ 1*b* (as long as the origin of $Pm\bar{3}m$ remains unchanged).

The concept of configuration equivalence may also be applied to types of Wyckoff set: two types of Wyckoff set are *configuration equivalent* if and only if for each crystallographic orbit belonging to the first type there exists a configuration-equivalent crystallographic orbit belonging to the second type of Wyckoff set, and *vice versa*. All types of Wyckoff set differ in their crystallographic orbits, but configuration-equivalent types of Wyckoff set result in the same set of point configurations.

A *lattice complex* is the set of all point configurations that correspond to the crystallographic orbits of a certain type of Wyckoff set.

There exist 402 classes of configuration-equivalent types of Wyckoff set and, therefore, 402 lattice complexes in $\mathbb{E}^3$.

Example

Let us consider again the type of Wyckoff set *P*4/*mmm* 4*l* to 4*o* (the last example in Section 3.4.1.2). The set of all corresponding point configurations constitutes a lattice complex. Its

point configurations may be derived as described above, but now – instead of starting from just a particular group – starting from all space groups of type $P4/mmm$ with all conceivable positions of the origins and lengths and orientations of the basis vectors. Accordingly, the point configurations may differ in their relative position in space, their orientation, and in the distances between the centres and the size of their squares.

Just as all crystal forms of a particular type may be related to different point-group types, the same lattice complex may occur in different space-group types.

Example

The lattice complex 'cubic primitive lattice' may be generated, among others, in $Pm\bar{3}m$ 1*a*, *b*, in $Fm\bar{3}m$ 8*c* and in $Ia\bar{3}$ 8*a*, *b* with site symmetry $m\bar{3}m$, $\bar{4}3m$ and $.\bar{3}.$, respectively. The type of Wyckoff set specified by $Pm\bar{3}m$ 1*a*, *b* leads to the same set of point configurations as $Fm\bar{3}m$ 8*c* or $Ia\bar{3}$ 8*a*, *b*. Each point configuration of this lattice complex can be generated by a properly chosen space group of each of these space-group types.

Configuration-equivalent crystallographic orbits do not necessarily belong to configuration-equivalent types of Wyckoff set.

Example

The orbits of the types of Wyckoff set $Pm\bar{3}m$ 1*a*, *b* and $Fm\bar{3}$ 8*c* both refer to the set of all conceivable primitive cubic point lattices. Therefore, these two types of Wyckoff set are configuration equivalent and are associated with the same lattice complex. The type of Wyckoff set *P*432 8*g* x, x, x, however, comprises apart from crystallographic orbits with $x = \frac{1}{4}$ also those with $x \neq \frac{1}{4}$. The orbits with $x = \frac{1}{4}$ refer to the same set of point configurations as $Pm\bar{3}m$ 1*a*, *b* and $Fm\bar{3}$ 8*c*, whereas those with $x \neq \frac{1}{4}$ give rise to point configurations with different properties. As a consequence, the type of Wyckoff set *P*432 8*g* x, x, x is not configuration equivalent with $Pm\bar{3}m$ 1*a*, *b* and $Fm\bar{3}$ 8*c*, and, therefore, belongs to another lattice complex.

As this example shows, lattice complexes do not form equivalence classes of point configurations, but a certain point configuration may belong to several lattice complexes.

As each type of Wyckoff set uniquely refers to a certain lattice complex, one can also assign all corresponding Wyckoff sets, Wyckoff positions and crystallographic orbits to that lattice complex. A certain lattice complex, however, is frequently related to different types of Wyckoff set.

Among the different types of Wyckoff set belonging to a certain lattice complex, one stands out because its crystallographic orbits show the highest site symmetry. This one is called the *characteristic type of Wyckoff set* of that lattice complex, and the corresponding space-group type its *characteristic space-group type*. All other types of Wyckoff set are referred to as non-characteristic. The term 'characteristic' may also be transferred to particular Wyckoff sets out of the characteristic type. The space groups of all the other types in which the lattice complex may be generated are subgroups of the space groups of its characteristic type.

Different lattice complexes may have the same characteristic space-group type, but then they differ in the oriented site symmetry of their Wyckoff positions within that space-group type.

The characteristic space-group type together with the oriented site symmetry expresses the common symmetry properties of all point configurations of a lattice complex and can be used for its identification. For the purpose of *reference symbols* of lattice complexes, however, instead of the site symmetry the Wyckoff letter of one of the Wyckoff positions with that site symmetry is arbitrarily chosen, as first done by Hermann (1935). This Wyckoff position is called the *characteristic Wyckoff position* of the lattice complex.

Example

$Pm\bar{3}m$ is the characteristic space-group type for the lattice complex of all cubic primitive point lattices. The Wyckoff positions with the highest possible site symmetry $m\bar{3}m$ are l*a* 0, 0, 0 and 1*b* $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$, from which 1*a* has been chosen as the characteristic position. Thus, the reference symbol of this lattice complex is $Pm\bar{3}m$ *a*.

Example

$Pm\bar{3}m$ is also the characteristic space-group type for a second lattice complex that corresponds to Wyckoff position 8*g* .3*m* x, x, x. The reference symbol for this lattice complex is $Pm\bar{3}m$ *g*. Each of its point configurations may be derived by replacing each point of a cubic primitive lattice by eight points arranged at the corners of a cube.

All types of Wyckoff set (together with their Wyckoff sets and Wyckoff positions) that generate, as described above, the same set of point configurations are assigned to the same lattice complex. Accordingly, the following criterion holds: two Wyckoff positions are assigned to the same lattice complex if there is a suitable transformation that maps the point configurations of the two Wyckoff positions onto each other and if their space groups belong to the same crystal family (*cf.* Section 1.3.4.4). Suitable transformations are translations, proper or improper rotations, isotropic or anisotropic expansions or more general affine mappings (without violation of the metric conditions for the corresponding crystal family), and all their products.

By this criterion, the Wyckoff positions of all space groups (1731 entries in the space-group tables, 1128 types of Wyckoff set) are uniquely assigned to 402 lattice complexes. This assignment was first done by Hermann in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935). The corresponding information has also been given by Fischer *et al.* (1973).

The same concept has been used for the point configurations and Wyckoff positions in the plane groups. Here the Wyckoff positions (72 entries in the plane-group tables, 51 types of Wyckoff set) are assigned to 30 plane lattice complexes or net complexes (*cf.* Burzlaff *et al.*, 1968). The complexes for the crystallographic subperiodic groups in three-dimensional space, *i.e.* for the crystallographic point groups, rod groups and layer groups, have been derived by Koch & Fischer (1978*a*).

3.4.1.4. Limiting complexes and comprehensive complexes

As has been shown above, lattice complexes define equivalence classes of orbits but not of point configurations. This property gave rise to the concept of limiting complexes and comprehensive complexes (Fischer & Koch, 1974*a*; Koch, 1974).

For morphological crystal forms an almost analogous situation exists. A certain tetragonal prism, for example, may be a general representative of the crystal form 'tetragonal prism' on the one hand or it may be a special representative of the crystal forms 'tetragonal pyramid' or 'tetragonal disphenoid' on the other hand. In the first case the generating point group may belong to the types $4/mmm$, 422, $4/m$ or $\bar{4}2m$ (with site symmetry 2 for each face), in the second case the types of the generating point group

are 4*mm* or 4 and $\bar{4}2m$ (site symmetry *m*) or $\bar{4}$, respectively. The crystal form 'tetragonal prism' is a limiting form of both crystal forms 'tetragonal pyramid' and 'tetragonal disphenoid'.

If a first lattice complex forms a true subset of a second one, *i.e.* if each point configuration of the first lattice complex also belongs to the second one, then the first one is called a *limiting complex* of the second one and the second complex is called a *comprehensive complex* of the first one (*cf.* Koch & Fischer, 1985).

Example

The cubic lattice complex $I\bar{4}3d$ 16*c* *x*, *x*, *x* involves two limiting complexes, namely $Im\bar{3}m$ 2*a* 0, 0, 0 and $Ia\bar{3}d$ 16*b* $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$. The orbits from $I\bar{4}3d$ 16*c* with $x = 0$ and from $Im\bar{3}m$ 2*a* are configuration equivalent, and so are the orbits from $I\bar{4}3d$ 16*c* with $x = \frac{1}{8}$ and from $Ia\bar{3}d$ 16*b*.

Example

The tetragonal lattice complex $I4_1/amd$ 4*a* is a comprehensive complex of the cubic complex $Fd\bar{3}m$ 8*a*. Each orbit of $Fd\bar{3}m$ 8*a* is configuration equivalent to a crystallographic orbit of a special space group of type $I4_1/amd$ with axial ratio $c/a = (2)^{1/2}$.

Furthermore, two lattice complexes without a limiting-complex relationship may have a non-empty intersection. Then the point configurations of the intersection result in one or, in very exceptional cases, in two or more other lattice complexes (*cf.* Koch, 1974).

Example

The intersection of the two lattice complexes $Im\bar{3}$ 24*g* and $I\bar{4}3m$ 24*g* consists of all point configurations belonging to $Im\bar{3}m$ 24*h*, *i.e.* each point configuration out of this intersection refers to an orbit from $Im\bar{3}m$ 24*h* 0, *x*, *x* and, in addition, to an orbit from $Im\bar{3}$ 24*g* 0, *y*, *z* with $y = z$ and to another one from $I\bar{4}3m$ 24*g* *x*, *x*, *z* with $z = 0$.

Example

The intersection of the trivariant lattice complexes $Fm\bar{3}c$ 192*j* and *P*432 24*k* consists of two bivariant limiting complexes, namely of $Pm\bar{3}m$ 24*k* 0, *y*, *z* and of $Pm\bar{3}m$ 24*m* *x*, *x*, *z*.

Each point configuration of a given lattice complex is uniquely related to two space groups: (1) the space group that reflects its eigensymmetry, and (2) a space group that belongs to the characteristic space-group type of the lattice complex under consideration. In most cases the two groups coincide. Only when the point configuration under consideration belongs to a limiting complex is the first group a proper supergroup of the second one.

Complete lists of the limiting complexes of all lattice complexes are not available. Koch (1974) derived the limiting complexes of the cubic lattice complexes. The limiting complexes that refer to specialized coordinate parameters may be derived from a table by Engel *et al.* (1984), who listed the respective non-characteristic orbits for all space-group types. The limiting complexes of the tetragonal and trigonal lattice complexes that are due to metrical specializations are tabulated by Koch & Fischer (2003) and by Koch & Sowa (2005), respectively.

Fischer & Koch (1978) tabulated the limiting complexes for the crystallographic point groups, rod groups and layer groups. As each type of plane group uniquely corresponds to a certain type of isomorphic layer group, information on the limiting complexes of the lattice complexes of the plane groups may easily be extracted from the respective table for the layer groups. This information may also be taken from a list of the non-characteristic orbits of the plane groups by Matsumoto & Wondratschek (1987).

3.4.1.5. Additional properties of lattice complexes

3.4.1.5.1. The degrees of freedom

Each Wyckoff position shows a certain number of coordinate parameters that can be varied independently. For most lattice complexes, this number is the same for any of its Wyckoff positions. For the lattice complex with characteristic Wyckoff position $Pm\bar{3}$ 12*j* *m*.. 0, *y*, *z*, for instance, this number is two. The lattice complex has two degrees of freedom. If, however, the variation of a certain coordinate corresponds to a shift of the point configuration as a whole, the lattice complex has fewer degrees of freedom than the Wyckoff position that is being considered. Therefore, $I4_1$ 8*b* *x*, *y*, *z* is the characteristic Wyckoff position of a lattice complex with only two degrees of freedom, although position 8*b* itself has three coordinate parameters that can be varied independently. The lattice complex *P*4/*m* *j* has two degrees of freedom and refers to Wyckoff positions with two as well as with three independent coordinate parameters, namely to *P*4/*m* 4*j* *m*.. *x*, *y*, 0 and to *P*4 4*d* 1 *x*, *y*, *z*.

According to its number of degrees of freedom, a lattice complex is called *invariant*, *univariant*, *bivariant* or *trivariant*. In total, there exist 402 lattice complexes, 36 of which are invariant, 106 univariant, 105 bivariant and 155 trivariant. The 30 plane lattice complexes are made up of 7 invariant, 10 univariant and 13 bivariant ones.

Most of the invariant and univariant lattice complexes correspond to several types of Wyckoff set. In contrast to that, only one type of Wyckoff set can belong to each trivariant lattice complex. A bivariant lattice complex may either correspond to one type of Wyckoff set (*e.g.* $Pm\bar{3}$ *j*) or to two types (*P*4 *d*, for example, belongs to the lattice complex with the characteristic Wyckoff position *P*4/*m* *j*).

3.4.1.5.2. Weissenberg complexes

Depending on their site-symmetry groups, two kinds of Wyckoff position may be distinguished:

(i) The site-symmetry group of any point is a proper subgroup of another site-symmetry group from the same space group. Then the Wyckoff position contains, among others, orbits where suitably chosen points may be infinitely close together.

Example

Each point configuration of the lattice complex with the characteristic Wyckoff position *P*4/*mmm* 4*j* *m*.2*m* *x*, *x*, 0 may be imagined as squares of four points surrounding the points of a tetragonal primitive lattice. For $x \rightarrow 0$, the squares become infinitesimally small. Orbits with $x = 0$ show site symmetry 4/*mmm*, their multiplicity is decreased from 4 to 1, and they belong to Wyckoff position *P*4/*mmm* 1*a*.

(ii) The site-symmetry group of every point belonging to the Wyckoff position under consideration is not a proper subgroup of any other site-symmetry group from the same space group.

Example

In *Pmma*, there does not exist a site-symmetry group that is a proper supergroup of *mm*2, the site symmetry of Wyckoff position *Pmma* 2*e* $\frac{1}{4}$, 0, *z*. As a consequence, the

Table 3.4.1.1
Reference symbols of the 31 Weissenberg complexes with $f \geq 1$ degrees of freedom in $\mathbb{E}^3$

Weissenberg complex	f	Weissenberg complex	f
$P2_1/m$ *e*	2	$I\bar{4}2d$ *d*	1
$P2/c$ *e*	1	$P4/nmm$ *c*	1
$C2/c$ *e*	1	$I4_1/acd$ *e*	1
$P2_12_12_1$ *a*	3	$P3_2$ *a*	2
Pmma e	1	$P3_212$ *a*	1
Pbcm d	2	$P3_221$ *a*	1
Pmmn a	1	$P\bar{3}m1$ *d*	1
Pnma c	2	$P6_1$ *a*	2
Cmcm c	1	$P6_122$ *a*	1
Cmme g	1	$P6_122$ *b*	1
Imma e	1	$P2_13$ *a*	1
$P4_3$ *a*	2	$I2_13$ *a*	1
$P4_322$ *a*	1	$I2_13$ *b*	1
$P4_322$ *c*	1	$Ia\bar{3}$ *d*	1
$P4_32_12$ *a*	1	$I\bar{4}3d$ *c*	1
$I4_122$ *f*	1		

distance between any two symmetry-equivalent points belonging to *Pmma e* cannot become shorter than the minimum of $\frac{1}{2}a$, *b* and *c*.

A lattice complex refers either to Wyckoff positions exclusively of the first or exclusively of the second kind. Most lattice complexes are related to Wyckoff positions of the first kind.

There exist, however, 67 lattice complexes without point configurations with infinitesimally short distances between symmetry-related points [*cf. Hauptgitter* (Weissenberg, 1925)]. These lattice complexes were called *Weissenberg complexes* by Fischer *et al.* (1973). The 36 invariant lattice complexes are trivial examples of Weissenberg complexes. The other 31 Weissenberg complexes with degrees of freedom (24 univariant, 6 bivariant, 1 trivariant) are compiled in Table 3.4.1.1. They have the following common property: each Weissenberg complex contains at least two invariant limiting complexes belonging to the same crystal family (see also Section 3.4.3.1.3).

Example

The Weissenberg complex *Pmma* $2e\ \frac{1}{4}, 0, z$ is a comprehensive complex of *Pmmm a* and of *Cmmm a*. Within the characteristic Wyckoff position, $\frac{1}{4}, 0, 0$ refers to *Pmmm a* and $\frac{1}{4}, 0, \frac{1}{4}$ to *Cmmm a*.

Apart from the seven invariant plane lattice complexes, there exists only one further Weissenberg complex within the plane groups, namely the univariant rectangular complex *p*2*mg c*.

3.4.2. The concept of characteristic and non-characteristic orbits, comparison with the lattice-complex concept

3.4.2.1. Definitions

The generating space group of any crystallographic orbit may be compared with the eigensymmetry of its point configuration. If both groups coincide, the orbit is called a *characteristic crystallographic orbit*, otherwise it is named a *non-characteristic crystallographic orbit* (Wondratschek, 1976; Engel *et al.*, 1984; see also Section 1.1.7). If the eigensymmetry group contains additional translations in comparison with those of the generating space group, the term *extraordinary orbit* is used (*cf.* also Matsumoto & Wondratschek, 1979). Each class of configuration-equivalent orbits contains exactly one characteristic crystallographic orbit.

The set of all point configurations in $\mathbb{E}^3$ can be divided into 402 equivalence classes by means of their eigensymmetry: two point configurations belong to the same *symmetry type of point configuration* if and only if their characteristic crystallographic orbits belong to the same type of Wyckoff set.

As each crystallographic orbit is uniquely related to a certain point configuration, each equivalence relationship on the set of all point configurations also implies an equivalence relationship on the set of all crystallographic orbits: two crystallographic orbits are assigned to the same *orbit type* (*cf.* also Engel *et al.*, 1984) if and only if the corresponding point configurations belong to the same symmetry type.

In contrast to lattice complexes, neither symmetry types of point configuration nor orbit types can be used to define equivalence relations on Wyckoff positions, Wyckoff sets or types of Wyckoff set. Two crystallographic orbits coming from the same Wyckoff position belong to different orbit types, if – owing to special coordinate values – they differ in the eigensymmetry of their point configurations. Furthermore, two crystallographic orbits with the same coordinate description, but stemming from different space groups of the same type, may belong to different orbit types because of a specialization of the metrical parameters.

Example

The eigensymmetry of orbits from Wyckoff position $P\bar{4}3m$ $4e$ x, x, x with $x = \frac{1}{4}$ or $x = \frac{3}{4}$ is enhanced to $Fm\bar{3}m$ $4a, b$ and hence they belong to a different orbit type to those with $x \neq \frac{1}{4}, \frac{3}{4}$.

Example

In general, an orbit belonging to the type of Wyckoff set $I4/m$ $2a, b$ corresponds to a point configuration with eigensymmetry $I4/mmm$ $2a, b$. If, however, the space group $I4/m$ has specialized metrical parameters, *e.g.* $c/a = 1$ or $c/a = 2^{1/2}$, then the eigensymmetry of the point configuration is enhanced to $Im\bar{3}m$ $2a$ or $Fm\bar{3}m$ $4a, b$, respectively.

3.4.2.2. Comparison of the concepts of lattice complexes and orbit types

It is the common intention of the lattice-complex and the orbit-type concepts to subdivide the point configurations and crystallographic orbits in $\mathbb{E}^3$ into subsets with certain common properties. With only a few exceptions, the two concepts result in different subsets. As similar but not identical symmetry considerations are used, each lattice complex is uniquely related to a certain symmetry type of point configuration and to a certain orbit type, and *vice versa*. Therefore, the two concepts result in the same number of subsets: there exist 402 lattice complexes and 402 symmetry types of point configuration and orbit types. The differences between the subsets are caused by the different properties of the point configurations and crystallographic orbits used for the classifications (*cf.* also Koch & Fischer, 1985).

The concept of orbit types is entirely based on the eigensymmetry of the particular point configurations: a crystallographic orbit is regarded as an isolated entity, *i.e.* detached from its Wyckoff position and its type of Wyckoff set. On the contrary, lattice complexes result from a hierarchy of classifications of crystallographic orbits into Wyckoff positions, Wyckoff sets, types of Wyckoff set and classes of configuration-equivalent types of

Table 3.4.2.1
Reference symbols of the 28 lattice complexes with $f \geq 1$ degrees of freedom without any limiting complex

Lattice complex	f	Lattice complex	f
*P*4/*mmm l*	1	*Pm*$\bar{3}$*n g*	1
*P*4$_2$/*mmc j*	1	*Pm*$\bar{3}$*n j*	1
*I*4/*mmm i*	1	*Pn*$\bar{3}$*m e*	1
*P*6$_2$22 *g*	1	*Pn*$\bar{3}$*m i*	1
*P*6/*mmm l*	1	*Fm*$\bar{3}$*m f*	1
*P*6/*mmm p*	2	*Fm*$\bar{3}$*m h*	1
*P*4$_2$32 *k*	1	*Fd*$\bar{3}$*m g*	2
*I*432 *i*	1	*Im*$\bar{3}$*m e*	1
*I*4$_1$32 *h*	1	*Im*$\bar{3}$*m f*	1
*I*4$_1$32 *i*	3	*Im*$\bar{3}$*m g*	1
Pm$\bar{3}$*m e*	1	*Im*$\bar{3}$*m i*	1
Pm$\bar{3}$*m i*	1	*Im*$\bar{3}$*m j*	2
Pm$\bar{3}$*m k*	2	*Im*$\bar{3}$*m l*	3
Pm$\bar{3}$*m m*	2	*Ia*$\bar{3}$*d e*	1

Wyckoff set, *i.e.* a crystallographic orbit is always considered as being embedded in its type of Wyckoff set, and the eigensymmetry of a particular point configuration is disregarded. The differences between the two concepts become clear if limiting complexes are considered.

Forty-nine lattice complexes without any limiting complex exist (*cf.* Table 3.4.2.1). They coincide completely with the corresponding symmetry types of point configurations. As can be extracted from the tables by Engel *et al.* (1984) there exist 15 additional lattice complexes without limiting complexes due to specialized coordinates. For fundamental reasons, no cubic or hexagonal complexes allow any metrical specialization.

Example

The lattice complex *P*$\bar{1}$ *a* of all triclinic point lattices includes as limiting complexes the 13 other lattice complexes that refer to Bravais lattices. Hence the crystallographic orbits of *P*$\bar{1}$ *a* belong to 14 different orbit types.

Example

The lattice complex *Fddd a* of all orthorhombic diamond patterns includes as limiting complexes those of the tetragonal and the cubic diamond patterns *I*4$_1$/*amd a* and *Fd*$\bar{3}$*m a*, respectively. The orbits of *Fddd a* with specialized metric, therefore, belong to the orbit types *I*4$_1$/*amd a* or *Fd*$\bar{3}$*m a*.

353 lattice complexes comprise at least one limiting complex. Each of them includes additional point configurations in comparison to the corresponding symmetry type of point configuration (and orbit type), namely those belonging to the limiting complex.

Example

Lattice complex *Im*$\bar{3}$ 24*g* 0, *y*, *z* comprises for $y = z$ the limiting complex *Im*$\bar{3}$*m* 24*h*, and for $y = z = \frac{1}{4}$ the limiting complex *Pm*$\bar{3}$*m* 3*c*. The corresponding orbits with $y = z$ and $y = z = \frac{1}{4}$ do not belong to orbit type *Im*$\bar{3}$ 24*g*.

Example

*P*4/*mmm* 8*r* *x*, *x*, *z* comprises for $z = \frac{1}{4}$ the limiting complex *P*4/*mmm* 4*j*, for $x = \frac{1}{4}$ the limiting complex *P*4/*mmm* 2*g*, for $x = z = \frac{1}{4}$ the limiting complex *P*4/*mmm* 1*a*, for $a = c$ and $x = z$ the limiting complex *Pm*$\bar{3}$*m* 8*g*, and for $a = c$ and $x = z = \frac{1}{4}$ the limiting complex *Pm*$\bar{3}$*m* l*a*. Again, none of the corresponding orbits belong to orbit type *P*4/*mmm* 8*r*.

The comparison of an orbit type with its corresponding lattice complex is more intricate. Again, the concept of limiting complexes and comprehensive complexes elucidates the interrelation.

Let *A* be a lattice complex with a limiting complex *B* and a comprehensive complex *C*. The respective orbit types will also be designated *A*, *B* and *C* (*e.g.* *A* = *Im*$\bar{3}$*m* 24*h* 0, *x*, *x*; *B* = *Pm*$\bar{3}$*m* 3*c*, *d* 0, $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$, 0, 0; *C* = *Im*$\bar{3}$ 24*g* 0, *y*, *z*). Then a crystallographic orbit from a Wyckoff position of lattice complex *A* belongs to orbit type *A* only if it does not correspond to a point configuration of the limiting complex *B* (*i.e.* only the crystallographic orbits of *Im*$\bar{3}$*m* 24*h* with $x \neq \frac{1}{4}$ belong to orbit type *Im*$\bar{3}$*m* 24*h*). The crystallographic orbits of lattice complex *A*, however, that do correspond to the limiting complex *B* belong to orbit type *B* (*i.e.* all crystallographic orbits from *Im*$\bar{3}$*m* 24*h* with $x = \frac{1}{4}$ belong to orbit type *Pm*$\bar{3}$*m* 3*c*, *d*). On the contrary, those orbits that refer to lattice complex *C* and that happen to correspond to the limiting complex *A* of *C* belong to orbit type *A* instead of orbit type *C*. All crystallographic orbits of *Im*$\bar{3}$ 24*g* 0, *y*, *z* with $y = z$ or $y = z = \frac{1}{4}$ create point configurations of lattice complex *Im*$\bar{3}$ 24*g* but belong to orbit type *Im*$\bar{3}$*m* 24*h* or *Pm*$\bar{3}$*m* 3*c*, *d*, respectively.

For the comparison of lattice complexes and orbit types the concept of non-characteristic orbits is less helpful than the concept of limiting complexes. In terms of lattice complexes, there exist two basically different reasons for a crystallographic orbit to be non-characteristic:

(1) The crystallographic orbit under consideration belongs to a non-characteristic type of Wyckoff set of a lattice complex. Then this orbit, together with all other orbits from its type of Wyckoff set, is non-characteristic. A characteristic crystallographic orbit necessarily stems from a characteristic Wyckoff set of a lattice complex.
(2) The crystallographic orbit under consideration stands out with respect to the eigensymmetry of its point configuration compared with the other orbits out of its type of Wyckoff sets, *i.e.* it corresponds to a limiting complex. Then this orbit, together with all other orbits referring to that limiting complex, is non-characteristic.

As a consequence, three kinds of non-characteristic orbits may be distinguished:

(1) those that belong to a non-characteristic Wyckoff set, but do not correspond to a limiting complex, *e.g.* all orbits from *Pm*$\bar{3}$ 6*e* to *h*;
(2) those that belong to a characteristic Wyckoff set, but correspond to a limiting complex, *e.g.* *Pm*$\bar{3}$*m* 8*g* *x*, *x*, *x* with $x = \frac{1}{4}$ or *P*4/*mmm* 1*a*, *b* with $a = c$;
(3) those that belong to a non-characteristic Wyckoff set and, in addition, correspond to a limiting complex, *e.g.* *Pm*$\bar{3}$ 8*i* *x*, *x*, *x* with $x = \frac{1}{4}$.

As these considerations illustrate, limiting complexes and non-characteristic orbits do not coincide and a statement by Engel (1983) proposing this correspondence, therefore, is not correct.

The concept of lattice complexes and limiting complexes on the one hand and of orbit types and non-characteristic orbits on the other hand are complementary in a certain sense: it is possible to derive all orbit types and all non-characteristic orbits from the complete knowledge of lattice complexes and limiting complexes and *vice versa*.

Engel *et al.* (1984) enumerated for all space-group types those non-characteristic orbits that refer to special coordinates, but they excluded all further ones that are based on specialized metrical parameters of the generating space groups or on the simultaneous specialization of metrical and coordinate parameters. A computer program which enables the determination of non-characteristic orbits is now available (*NONCHAR* on the Bilbao Crystallographic Server at http://www.cryst.ehu.es). Lawrenson & Wondratschek (1976) listed the extraordinary orbits of the plane groups, and Matsumoto & Wondratschek (1987) listed the non-characteristic orbits of the plane groups.

The special, but not exceptional, case in which a non-characteristic orbit is produced only if both the coordinates *and* metric are specialized deserves extra concern. The crystallographic orbits from $R\bar{3}$ 6*f* x, y, z with $x = \frac{1}{4}, y = 0, z = \frac{1}{2}$ or $x = \frac{1}{4}, y = \frac{1}{2}, z = 0$ and with the rhombohedral angle $\alpha = 90°$ may be used as an example. The eigensymmetry of the corresponding point configurations is $Pm\bar{3}n$ 6*c*, *d* (corresponding to the position of the Cr atoms in the crystal structure of Cr_3Si). Accordingly, the lattice complex $R\bar{3}$ *f* comprises $Pm\bar{3}n$ *c* as limiting complex. $Pm\bar{3}n$ *c* shows special integral reflection conditions (*hkl*: $h + k + l = 2n$ or $h = 2n + 1$, $k = 4n$, $l = 4n + 2$; h, k, l permutable), which of course hold for all orbits of that type, *i.e.* also for the special orbits from $R\bar{3}$ *f* described above. As geometrical structure factors are independent of metrical parameters, these reflection conditions are even valid for crystallographic orbits from $R\bar{3}$ *f* with $a \neq 90°$ if the coordinates are restricted to $\frac{1}{4}, 0, \frac{1}{2}$ or to $\frac{1}{4}, \frac{1}{2}, 0$.

In general, the following statement holds: if a lattice complex causes special reflection conditions then exactly these conditions are also valid for any crystallographic orbit that refers to a comprehensive complex of that lattice complex if, in addition, this crystallographic orbit may be described by the same coordinate triplets as an orbit of the lattice complex under consideration.

3.4.3. Descriptive lattice-complex symbols and the assignment of Wyckoff positions to lattice complexes

3.4.3.1. Descriptive symbols

3.4.3.1.1. Introduction

For the study of relations between crystal structures, lattice-complex symbols are desirable that show as many relations between point configurations as possible. To this end, Hermann (1960) derived descriptive lattice-complex symbols that were further developed by Donnay *et al.* (1966) and completed by Fischer *et al.* (1973). These symbols describe the arrangements of the points in the point configurations and refer directly to the coordinate descriptions of the Wyckoff positions. Since a lattice complex, in general, contains Wyckoff positions with different coordinate descriptions, it may be represented by several different descriptive symbols. The symbols are further affected by the settings of the space group. The present section is restricted to the fundamental features of the descriptive symbols. Details have been described by Fischer *et al.* (1973). Tables 3.4.3.2 and 3.4.3.3 give for each Wyckoff position of a plane group or a space group, respectively, the multiplicity, the Wyckoff letter, the oriented site symmetry, the reference symbol of the corresponding lattice complex and the descriptive symbol.[4] The comparatively short descriptive symbols condense complicated verbal descriptions of the point configurations of lattice complexes.

[4] Some of the descriptive symbols listed in Table 3.4.3.3 differ slightly from those derived by Fischer *et al.* (1973) and used in editions of *International Tables for Crystallography* Volume A before 2002.

Table 3.4.3.1
Descriptive symbols of invariant lattice complexes in their characteristic Wyckoff position

Descriptive symbol	Crystal family	Characteristic Wyckoff position
C	*o* *m*	*Cmmm a* *C*2/*m a*
D	*c* *o*	*Fd*$\bar{3}$*m a* *Fddd a*
^{v}D	*t*	$I4_1/amd$ *a*
E	*h*	$P6_3/mmc$ *c*
F	*c* *o*	*Fm*$\bar{3}$*m a* *Fmmm a*
G	*h*	*P*6/*mmm c*
I	*c* *t* *o*	*Im*$\bar{3}$*m a* *I*4/*mmm a* *Immm a*
J	*c*	*Pm*$\bar{3}$*m c*
*J**	*c*	*Im*$\bar{3}$*m b*
M	*h*	*R*$\bar{3}$*m e*
N	*h*	*P*6/*mmm f*
P	*c* *h* *t* *o* *m* *a*	*Pm*$\bar{3}$*m a* *P*6/*mmm a* *P*4/*mmm a* *Pmmm a* *P*2/*m a* *P*$\bar{1}$ *a*
^{+}Q	*h*	$P6_222$ *c*
R	*h*	*R*$\bar{3}$*m a*
S	*c*	*I*$\bar{4}$3*d a*
*S**	*c*	*Ia*$\bar{3}$*d d*
T	*c* *o*	*Fd*$\bar{3}$*m c* *Fddd c*
^{v}T	*t*	$I4_1/amd$ *c*
^{+}V	*c*	$I4_132$ *c*
*V**	*c*	*Ia*$\bar{3}$*d c*
W	*c*	*Pm*$\bar{3}$*n c*
*W**	*c*	*Im*$\bar{3}$*m d*
^{+}Y	*c*	$P4_332$ *a*
$^{+}Y^{*}$	*c*	$I4_132$ *a*
*Y***	*c*	*Ia*$\bar{3}$*d b*

3.4.3.1.2. Invariant lattice complexes

An invariant lattice complex in its characteristic Wyckoff position is represented by a capital letter (sometimes in combination with a superscript). The first column of Table 3.4.3.1 gives a complete list of these symbols in alphabetical order. The characteristic Wyckoff positions are shown in column 3. Lattice complexes from different crystal families but with the same coordinate description for their characteristic Wyckoff positions receive the same descriptive symbol. If necessary, the crystal family may be stated explicitly by a small letter (column 2) preceding the lattice-complex symbol: *c* cubic, *t* tetragonal, *h* hexagonal, *o* orthorhombic, *m* monoclinic, *a* anorthic (triclinic).

Example

D is the descriptive symbol of the invariant cubic lattice complex $Fd\bar{3}m$ *a* as well as of the orthorhombic lattice complex *Fddd a*. The cubic lattice complex *cD* contains – among others – the point configurations corresponding to the arrangement of carbon atoms in diamond and of silicon atoms in β-cristobalite. The orthorhombic complex *oD* is a comprehensive complex of *cD*. It consists of all those point configurations that may be produced by orthorhombic deformations of the point configurations of *cD*.

The descriptive symbol of a non-characteristic Wyckoff position depends on the difference between the coordinate descriptions of the respective characteristic Wyckoff position and the position under consideration. Three cases may be distinguished, which may also occur in combinations.

(i) The two coordinate descriptions differ by an origin shift. Then, the respective shift vector is added as a prefix to the descriptive symbol of the characteristic Wyckoff position.

Example

The orthorhombic invariant lattice complex *F* is represented in its characteristic Wyckoff position *Fmmm a* by the coordinate triplets $0,0,0$; $\frac{1}{2},\frac{1}{2},0$; $0,\frac{1}{2},\frac{1}{2}$ and $\frac{1}{2},0,\frac{1}{2}$. In *Pnnn e* (origin choice 1), it is described by $\frac{1}{4},\frac{1}{4},\frac{1}{4}$; $\frac{3}{4},\frac{3}{4},\frac{1}{4}$; $\frac{1}{4},\frac{3}{4},\frac{3}{4}$ and $\frac{3}{4},\frac{1}{4},\frac{3}{4}$ and, therefore, receives the descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}F$.

(ii) The multiplicity of the Wyckoff position considered is higher than that of the corresponding characteristic position. Then, the coordinate description of this Wyckoff position can be transformed into that of the characteristic position by taking shorter basis vectors. Reduction of all three basis vectors by a factor of 2 is denoted by the subscript 2 on the descriptive symbol. Reduction of one or two basis vectors by a factor of 2 is denoted by one of the subscripts *a*, *b* or *c* or a combination of these. The subscript *C* means a factor of 3, *cc* a factor of 4 and *Cc* a factor of 6.

Examples

The characteristic Wyckoff position of the orthorhombic lattice complex *P* is *Pmmm a* with coordinate description $0,0,0$. This complex occurs also in *Pmma a* with coordinate triplets $0,0,0$; $\frac{1}{2},0,0$, and in *Pcca a* with $0,0,0$; $0,0,\frac{1}{2}$; $\frac{1}{2},0,0$; $\frac{1}{2},0,\frac{1}{2}$. The corresponding descriptive symbols are P_a and P_{ac}, respectively.

(iii) The coordinate description of a given Wyckoff position is related to that of the characteristic position by inversion or rotation of the coordinate system. Changing the superscript + into − in the descriptive symbol means that the Wyckoff position considered is mapped onto the characteristic position by an inversion through the origin, *i.e.* the two Wyckoff positions are enantiomorphic. A prime preceding the capital letter denotes that a 180° rotation is required.

Examples

(1) $^{+}Y^{*}$ is the descriptive symbol of the invariant lattice complex $I4_132$ *a* in its characteristic position. Wyckoff position $I4_132$ *b* with the descriptive symbol $^{-}Y^{*}$ belongs to the same lattice complex. The point configurations of $I4_132$ *a* and $I4_132$ *b* are enantiomorphic.

(2) *R* is the descriptive symbol of the invariant lattice complex formed by all rhombohedral point lattices. Its characteristic position $R\bar{3}m$ *a* corresponds to the coordinate triplets $0,0,0$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$. The same lattice complex is symbolized by $'R_c$ in the non-characteristic position $R\bar{3}c$ *b* with coordinate description $0,0,0$; $0,0,\frac{1}{2}$; $\frac{2}{3},\frac{1}{3},\frac{1}{3}$; $\frac{2}{3},\frac{1}{3},\frac{5}{6}$; $\frac{1}{3},\frac{2}{3},\frac{2}{3}$; $\frac{1}{3},\frac{2}{3},\frac{1}{6}$.

In non-characteristic Wyckoff positions, the descriptive symbols *P* and *I* may be replaced by *C* and *F*, respectively (tetragonal system), *C* by *A* or *B* (orthorhombic system), and *C* by *A*, *B*, *I* or *F* (monoclinic system). If the lattice complexes of rhombohedral space groups are described in rhombohedral coordinate systems, the symbols *R*, $'R_c$, *M* and $'M_c$ of the hexagonal description are replaced by *P*, *I*, *J* and J^{*}, respectively (preceded by the letter *r*, if necessary, to distinguish them from the analogous cubic invariant lattice complexes).

3.4.3.1.3. Lattice complexes with degrees of freedom

The descriptive symbols of lattice complexes with degrees of freedom consist, in general, of four parts: the shift vector, the distribution symmetry, the central part and the site-set symbol. Either of the first two parts may be absent.

Example

$0\frac{1}{2}0$ ..2 *C*4*xxz* is the descriptive symbol of the lattice complex $P4/nbm$ *m* in its characteristic position: $0\frac{1}{2}0$ is the shift vector, ..2 the distribution symmetry, *C* the central part and 4*xxz* the site-set symbol.

Normally, the central part is the symbol of an invariant lattice complex. The shift vector and central part together should be interpreted as described in Section 3.4.3.1.2. The point configurations of the Wyckoff position being considered can be derived from that described by the central part by replacing each point by a finite set of points, the site set. All points of a site set are symmetry-equivalent under the site-symmetry group of the point that they replace. A site set is symbolized by a string of numbers and letters. The product of the numbers gives the number of points in the site set, whereas the letters supply information on the pattern formed by these points. Site sets replacing different points may be differently oriented. In this case, the distribution-symmetry part of the reference symbol shows symmetry operations that relate such site sets to one another. The orientation of the corresponding symmetry elements is indicated as in the oriented site-symmetry symbols (*cf.* Section 2.2.12). If all site sets have the same orientation, no distribution symmetry is given.

Examples

(1) *I*4*xxx* ($I\bar{4}3m$ 8*c* x,x,x) designates a lattice complex, the point configurations of which are composed of tetrahedra 4*xxx* in parallel orientation replacing the points of a cubic body-centred lattice *I*. The vertices of these tetrahedra are located on body diagonals.

(2) ..2 *I*4*xxx* ($Pn\bar{3}m$ 8*e* x,x,x) represents the lattice complex for which, in contrast to the first example, the tetrahedra 4*xxx* around $0,0,0$ and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ differ in their orientation. They are related by a twofold rotation ..2 .

(3) $00\frac{1}{4}$ P_c4x is the descriptive symbol of Wyckoff position $P4_2/mcm$ 8*l* $x,0,\frac{1}{4}$. Each corresponding point configuration consists of squares of points 4*x* replacing the points of a tetragonal primitive lattice *P*. In comparison with *P*4*x*, $00\frac{1}{4}$ P_c4x shows a unit-cell enlargement by $\mathbf{c}' = 2\mathbf{c}$ and a subsequent shift by $0,0,\frac{1}{4}$.

In the case of a Weissenberg complex (*cf.* Section 3.4.1.5.2; Weissenberg, 1925; Fischer *et al.*, 1973), the central part of the descriptive symbol always consists of two (or more) symbols of invariant lattice complexes belonging to the same crystal family and forming limiting complexes of the Weissenberg complex under consideration. The shift vector then refers to the first limiting complex. The corresponding site-set symbols are distinguished by containing the number 1 as the only number, *i.e.* each site set consists of only one point.

Example

In $\frac{1}{4}00$ .2. P_aB1z (*Pmma* 2*e* $\frac{1}{4}, 0, z$), each of the two points $\frac{1}{4}, 0, 0$ and $\frac{3}{4}, 0, 0$, represented by $\frac{1}{4}00$ P_a, is replaced by a site set $1z$ containing only one point, *i.e.* the points of $\frac{1}{4}00$ P_a are shifted along the z axis. The shifts of the two points are related by a twofold rotation .2., *i.e.* are running in opposite directions. The point configurations of the two limiting complexes P_a and B refer to the special parameter values $z = 0$ and $z = \frac{1}{4}$, respectively.

The central parts of some lattice complexes with two or three degrees of freedom are formed by the descriptive symbol of a univariant Weissenberg complex instead of that of an invariant lattice complex. This is the case only if the corresponding characteristic space-group type does not refer to a suitable invariant lattice complex.

Example

In $\frac{1}{4}00$ .2. P_aB1z2y (*Pmma* 4*k* $\frac{1}{4}, y, z$), each of the two points $\frac{1}{4}, 0, z$ and $\frac{3}{4}, 0, \bar{z}$, represented by $\frac{1}{4}00$ .2. P_aB1z, is replaced by a site set $2y$ of two points forming a dumbbell. These dumbbells are oriented parallel to the y axis.

The symbol of a non-characteristic Wyckoff position is deduced from that of the characteristic position. The four parts of the descriptive symbol are subjected to the transformation necessary to map the characteristic Wyckoff position onto the Wyckoff position under consideration.

Example

The lattice complex with characteristic Wyckoff position *Imma* 8*h* $0, y, z$ has the descriptive symbol .2. B_b2yz for this position. Another Wyckoff position of this lattice complex is *Imma* 8*i* $x, \frac{1}{4}, z$. The corresponding point configurations are mapped onto each other by interchanging positive x and negative y directions and shifting by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$. Therefore, the descriptive symbol for Wyckoff position *Imma i* is $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 2.. A_a2xz.

In some cases, the Wyckoff position described by a lattice-complex symbol has more degrees of freedom than the lattice complex (see Section 3.4.1.5.1). In such cases, a letter (or a string of letters) in brackets is added to the symbol.

Examples

tP[*z*] for *P*4 *a*, *aP*[*xyz*] for *P*1 *a*.

3.4.3.1.4. Properties of the descriptive symbols

Different kinds of relations between lattice complexes are brought out.

Examples

$P \leftrightarrow P4x \leftrightarrow P4x2z$, $\quad I4xxx \leftrightarrow ..2\ I4xxx$, $\quad P4x \leftrightarrow I4x$.

In many cases, limiting-complex relations can be deduced from the symbols. This applies to limiting complexes due either to special metrical parameters (*e.g.* $cP \leftrightarrow rP$ *etc.*) or to special values of coordinates (*e.g.* both *P*4*x* and *P*4*xx* are limiting complexes of *P*4*xy*). If the site set consists of only one point, the central part of the symbol specifies all corresponding limiting complexes without degrees of freedom that are due to special values of the coordinates (*e.g.* 2_12_1. $FA_aB_bC_cI_aI_bI_c1xyz$ for the general position of $P2_12_12_1$).

3.4.3.2. Assignment of Wyckoff positions to Wyckoff sets and to lattice complexes

In Tables 3.4.3.2 and 3.4.3.3, the Wyckoff positions of all plane and space groups, respectively, are listed. Each Wyckoff position is identified by its Wyckoff letter together with its oriented site-symmetry symbol. It is assigned to its lattice complex by means of the reference symbol (*cf.* Section 3.4.1.3). Characteristic Wyckoff positions are marked by asterisks (*e.g.* 2*e* in $P2/c$). If in a particular space group several Wyckoff positions belong to the same Wyckoff set (*cf.* Sections 1.4.4.3 and 3.4.1.2; Koch & Fischer, 1975), the reference symbol is given only once (*e.g.* Wyckoff positions 4*l* to 4*o* in $P4/mmm$). To enable this, the usual sequence of Wyckoff positions had to be changed in a few cases (*e.g.* in $P4_2/mcm$). For Wyckoff positions assigned to the same lattice complex but belonging to different Wyckoff sets, the reference symbol is repeated. In $I4/m$, for example, Wyckoff positions 4*c* and 4*d* are both assigned to the lattice complex $P4/mmm\ a$. They do not belong, however, to the same Wyckoff set because the site-symmetry groups $2/m$.. of 4*c* and $\bar{4}$.. of 4*d* are different.

The last columns of Tables 3.4.3.2 and 3.4.3.3 show the descriptive lattice-complex symbol for each Wyckoff position.

3.4.4. Applications of the lattice-complex concept

3.4.4.1. Geometrical properties of point configurations

To study the geometrical properties of all point configurations in three-dimensional space, it is not necessary to consider all Wyckoff positions of the space groups or all 1128 types of Wyckoff set. Instead, one may restrict the investigations to the characteristic Wyckoff positions of the 402 lattice complexes. The results can then be transferred to all non-characteristic Wyckoff positions of the lattice complexes, as listed in Tables 3.4.3.2 and 3.4.3.3.

The determination of all types of sphere packings with cubic and tetragonal symmetry forms an example for this kind of procedure (Fischer, 1973, 1974, 1991*a*,*b*, 1993). The cubic lattice complex *I*4*xxx*, for example, allows two types of sphere packings within its characteristic Wyckoff position $I\bar{4}3m$ 8*c* .3*m*. x, x, x. Sphere packings with three-membered rings and nine contacts per sphere are formed if $x = 3/16$. The parameter region $3/16 < x < \frac{1}{4}$ corresponds to sphere packings with four-membered rings and six contacts per sphere (*cf.* Fischer, 1973). Ag_3PO_4 crystallizes with symmetry $P\bar{4}3n$ (Deschizeaux-Cheruy *et al.*, 1982) and the oxygen atoms occupy Wyckoff position 8*e* .3. x, x, x, which also belongs to lattice complex *I*4*xxx*. Comparison of the coordinate parameter x = 0.1491 for the oxygen atoms with the sphere-packing parameters listed for $I\bar{4}3m\ c$ shows directly that the oxygen arrangement in this crystal structure does not form a sphere packing.

Other examples for this approach are the derivation of crystal potentials (Naor, 1958), of coordinate restrictions in

(*continued on page* 823)

Table 3.4.3.2
Plane groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes

Wyckoff positions of the same Wyckoff set can be recognized by their consecutive listing without repetition of the reference symbol. Characteristic Wyckoff sets are marked by asterisks.

1 *p*1

1	*a*	1		*p*2 *a*	$P[xy]$

2 *p*2

1	*a*	2	*	*p*2 *a*	P
1	*b*				$0\frac{1}{2}$ P
1	*c*				$\frac{1}{2}0$ P
1	*d*				$\frac{1}{2}\frac{1}{2}$ P
2	*e*	1	*	*p*2 *e*	$P2xy$

3 *pm*

1	*a*	*.m.*		*p*2*mm a*	$P[y]$
1	*b*				$\frac{1}{2}0$ $P[y]$
2	*c*	1		*p*2*mm e*	$P2x[y]$

4 *pg*

2	*a*	1		*p*2*mg c*	$2..$ $P_bC1x[y]$

5 *cm*

2	*a*	*.m.*		*c*2*mm a*	$C[y]$
4	*b*	1		*c*2*mm d*	$C2x[y]$

6 *p*2*mm*

1	*a*	2*mm*	*	*p*2*mm a*	P
1	*b*				$0\frac{1}{2}$ P
1	*c*				$\frac{1}{2}0$ P
1	*d*				$\frac{1}{2}\frac{1}{2}$ P
2	*e*	*..m*	*	*p*2*mm e*	$P2x$
2	*f*				$0\frac{1}{2}$ $P2x$
2	*g*	*.m.*			$P2y$
2	*h*				$\frac{1}{2}0$ $P2y$
4	*i*	1	*	*p*2*mm i*	$P2x2y$

7 *p*2*mg*

2	*a*	2..		*p*2*mm a*	P_a
2	*b*				$0\frac{1}{2}$ P_a
2	*c*	*.m.*	*	*p*2*mg c*	$\frac{1}{4}0$ $2..$ P_aC1y
4	*d*	1	*	*p*2*mg d*	$.m.$ P_a2xy

8 *p*2*gg*

2	*a*	2..		*c*2*mm a*	C
2	*b*				$\frac{1}{2}0$ C
4	*c*	1	*	*p*2*gg c*	$.g.$ $C2xy$

9 *c*2*mm*

2	*a*	2*mm*	*	*c*2*mm a*	C
2	*b*				$0\frac{1}{2}$ C
4	*c*	2..		*p*2*mm a*	$\frac{1}{4}\frac{1}{4}$ P_{ab}
4	*d*	*..m*	*	*c*2*mm d*	$C2x$
4	*e*	*.m.*			$C2y$
8	*f*	1	*	*c*2*mm f*	$C2x2y$

10 *p*4

1	*a*	4..		*p*4*mm a*	P
1	*b*				$\frac{1}{2}\frac{1}{2}$ P
2	*c*	2..		*p*4*mm a*	$0\frac{1}{2}$ C
4	*d*	1	*	*p*4 *d*	$P4xy$

11 *p*4*mm*

1	*a*	4*mm*	*	*p*4*mm a*	P
1	*b*				$\frac{1}{2}\frac{1}{2}$ P
2	*c*	2*mm.*		*p*4*mm a*	$0\frac{1}{2}$ C
4	*d*	*.m.*	*	*p*4*mm d*	$P4x$
4	*e*				$\frac{1}{2}\frac{1}{2}$ $P4x$
4	*f*	*..m*	*	*p*4*mm f*	$P4xx$
8	*g*	1	*	*p*4*mm g*	$P4x2y$

12 *p*4*gm*

2	*a*	4..		*p*4*mm a*	C
2	*b*	2.*mm*		*p*4*mm a*	$0\frac{1}{2}$ C
4	*c*	*..m*	*	*p*4*gm c*	$0\frac{1}{2}$ $.g.$ $C2xx$
8	*d*	1	*	*p*4*gm d*	$..m$ $C4xy$

13 *p*3

1	*a*	3..		*p*6*mm a*	P
1	*b*				$\frac{1}{3}\frac{2}{3}$ P
1	*c*				$\frac{2}{3}\frac{1}{3}$ P
3	*d*	1	*	*p*3 *d*	$P3xy$

14 *p*3*m*1

1	*a*	3*m.*		*p*6*mm a*	P
1	*b*				$\frac{1}{3}\frac{2}{3}$ P
1	*c*				$\frac{2}{3}\frac{1}{3}$ P
3	*d*	*.m.*	*	*p*3*m*1 *d*	$P3x\bar{x}$
6	*e*	1	*	*p*3*m*1 *e*	$P3x\bar{x}2y$

15 *p*31*m*

1	*a*	3.*m*		*p*6*mm a*	P
2	*b*	3..		*p*6*mm b*	G
3	*c*	*..m*	*	*p*31*m c*	$P3x$
6	*d*	1	*	*p*31*m d*	$P3x2y$

16 *p*6

1	*a*	6..		*p*6*mm a*	P
2	*b*	3..		*p*6*mm b*	G
3	*c*	2..		*p*6*mm c*	N
6	*d*	1	*	*p*6 *d*	$P6xy$

17 *p*6*mm*

1	*a*	6*mm*	*	*p*6*mm a*	P
2	*b*	3*m.*	*	*p*6*mm b*	G
3	*c*	2*mm*	*	*p*6*mm c*	N
6	*d*	*..m*	*	*p*6*mm d*	$P6x$
6	*e*	*.m.*	*	*p*6*mm e*	$P6x\bar{x}$
12	*f*	1	*	*p*6*mm f*	$P6x2y$

Table 3.4.3.3
Space groups: assignment of Wyckoff positions to Wyckoff sets and to lattice complexes

Wyckoff positions of the same Wyckoff set can be recognized by their consecutive listing without repetition of the reference symbol. Characteristic Wyckoff sets are marked by asterisks.

1 *P*1

1	*a*	1		$P\bar{1}$ *a*	*P*[*xyz*]

2 *P*$\bar{1}$

1	*a*	$\bar{1}$	*	$P\bar{1}$ *a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
1	*c*				$0\frac{1}{2}0$ *P*
1	*d*				$\frac{1}{2}00$ *P*
1	*e*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*f*				$\frac{1}{2}0\frac{1}{2}$ *P*
1	*g*				$0\frac{1}{2}\frac{1}{2}$ *P*
1	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*i*	1	*	$P\bar{1}$ *i*	*P*2*xyz*

3 *P*2

1	*a*	2		*P*2/*m a*	*P*[*y*]
1	*b*				$00\frac{1}{2}$ *P*[*y*]
1	*c*				$\frac{1}{2}00$ *P*[*y*]
1	*d*				$\frac{1}{2}0\frac{1}{2}$ *P*[*y*]
2	*e*	1		*P*2/*m m*	*P*2*xz*[*y*]

4 *P*2$_1$

2	*a*	1		$P2_1/m$ *e*	2_1 $P_bACI1xz$[*y*]

5 *C*2

2	*a*	2		*C*2/*m a*	*C*[*y*]
2	*b*				$00\frac{1}{2}$ *C*[*y*]
4	*c*	1		*C*2/*m i*	*C*2*xz*[*y*]

6 *Pm*

1	*a*	*m*		*P*2/*m a*	*P*[*xz*]
1	*b*				$0\frac{1}{2}0$ *P*[*xz*]
2	*c*	1		*P*2/*m i*	*P*2*y*[*xz*]

7 *Pc*

2	*a*	1		*P*2/*c e*	*c* P_cA1y[*xz*]

8 *Cm*

2	*a*	*m*		*C*2/*m a*	*C*[*xz*]
4	*b*	1		*C*2/*m g*	*C*2*y*[*xz*]

9 *Cc*

4	*a*	1		*C*2/*c e*	$\bar{1}$ C_cF1y[*xz*]

10 *P*2/*m*

1	*a*	2/*m*	*	*P*2/*m a*	*P*
1	*b*				$0\frac{1}{2}0$ *P*
1	*c*				$00\frac{1}{2}$ *P*
1	*d*				$\frac{1}{2}00$ *P*
1	*e*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*f*				$0\frac{1}{2}\frac{1}{2}$ *P*
1	*g*				$\frac{1}{2}0\frac{1}{2}$ *P*
1	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*i*	2	*	*P*2/*m i*	*P*2*y*
2	*j*				$\frac{1}{2}00$ *P*2*y*
2	*k*				$00\frac{1}{2}$ *P*2*y*
2	*l*				$\frac{1}{2}0\frac{1}{2}$ *P*2*y*
2	*m*	*m*	*	*P*2/*m m*	*P*2*xz*
2	*n*				$0\frac{1}{2}0$ *P*2*xz*
4	*o*	1	*	*P*2/*m o*	*P*2*xz*2*y*

11 *P*2$_1$/*m*

2	*a*	$\bar{1}$		*P*2/*m a*	P_b
2	*b*				$\frac{1}{2}00$ P_b
2	*c*				$00\frac{1}{2}$ P_b
2	*d*				$\frac{1}{2}0\frac{1}{2}$ P_b
2	*e*	*m*	*	$P2_1/m$ *e*	$0\frac{1}{4}0$ $2_1P_bACI1xz$
4	*f*	1	*	$P2_1/m$ *f*	*m* P_b2*xyz*

12 *C*2/*m*

2	*a*	2/*m*	*	*C*2/*m a*	*C*
2	*b*				$0\frac{1}{2}0$ *C*
2	*c*				$00\frac{1}{2}$ *C*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e*	$\bar{1}$		*P*2/*m a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	2	*	*C*2/*m g*	*C*2*y*
4	*h*				$00\frac{1}{2}$ *C*2*y*
4	*i*	*m*	*	*C*2/*m i*	*C*2*xz*
8	*j*	1	*	*C*2/*m j*	*C*2*xz*2*y*

13 *P*2/*c*

2	*a*	$\bar{1}$		*P*2/*m a*	P_c
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*				$0\frac{1}{2}0$ P_c
2	*d*				$\frac{1}{2}00$ P_c
2	*e*	2	*	*P*2/*c e*	$00\frac{1}{4}$ *c* P_cA1y
2	*f*				$\frac{1}{2}0\frac{1}{4}$ *c* P_cA1y
4	*g*	1	*	*P*2/*c g*	2 P_c2*xyz*

14 *P*2$_1$/*c*

2	*a*	$\bar{1}$		*C*2/*m a*	*A*
2	*b*				$\frac{1}{2}00$ *A*
2	*c*				$00\frac{1}{2}$ *A*
2	*d*				$\frac{1}{2}0\frac{1}{2}$ *A*
4	*e*	1	*	$P2_1/c$ *e*	*c* *A*2*xyz*

15 *C*2/*c*

4	*a*	$\bar{1}$		*C*2/*m a*	C_c
4	*b*				$0\frac{1}{2}0$ C_c
4	*c*				$\frac{1}{4}\frac{1}{4}0$ *F*
4	*d*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ *F*
4	*e*	2	*	*C*2/*c e*	$00\frac{1}{4}$ $\bar{1}$ C_cF1y
8	*f*	1	*	*C*2/*c f*	2_1 C_c2*xyz*

Table 3.4.3.3 (continued)

16 *P*222

1	*a*	222		*Pmmm a*	*P*
1	*b*				$\frac{1}{2}00$ *P*
1	*c*				$0\frac{1}{2}0$ *P*
1	*d*				$00\frac{1}{2}$ *P*
1	*e*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*f*				$\frac{1}{2}0\frac{1}{2}$ *P*
1	*g*				$0\frac{1}{2}\frac{1}{2}$ *P*
1	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*i*	2..		*Pmmm i*	*P*2*x*
2	*j*				$00\frac{1}{2}$ *P*2*x*
2	*k*				$0\frac{1}{2}0$ *P*2*x*
2	*l*				$0\frac{1}{2}\frac{1}{2}$ *P*2*x*
2	*m*	.2.			*P*2*y*
2	*n*				$00\frac{1}{2}$ *P*2*y*
2	*o*				$\frac{1}{2}00$ *P*2*y*
2	*p*				$\frac{1}{2}0\frac{1}{2}$ *P*2*y*
2	*q*	..2			*P*2*z*
2	*r*				$\frac{1}{2}00$ *P*2*z*
2	*s*				$0\frac{1}{2}0$ *P*2*z*
2	*t*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*u*	1	*	*P*222 *u*	*P*2*x*2*yz*

17 $P222_1$

2	*a*	2..		*Pmma e*	.2. P_cB1x
2	*b*				$0\frac{1}{2}0$ .2. P_cB1x
2	*c*	.2.			$00\frac{1}{4}$ 2.. P_cA1y
2	*d*				$\frac{1}{2}0\frac{1}{4}$ 2.. P_cA1y
4	*e*	1	*	$P222_1$ *e*	.2. $P_cB1x2yz$

18 $P2_12_12$

2	*a*	..2		*Pmmn a*	2_1.. *CI*1*z*
2	*b*				$0\frac{1}{2}0$ 2_1.. *CI*1*z*
4	*c*	1	*	$P2_12_12$ *c*	2_1.. *CI*1*z*2*xy*

19 $P2_12_12_1$

4	*a*	1	*	$P2_12_12_1$ *a*	2_12_1. $FA_aB_bC_cI_aI_bI_c1xyz$

20 $C222_1$

4	*a*	2..		*Cmcm c*	.2_1. C_cF1x
4	*b*	.2.			$00\frac{1}{4}$ 2_1.. C_cF1y
8	*c*	1	*	$C222_1$ *c*	.2_1. $C_cF1x2yz$

21 *C*222

2	*a*	222		*Cmmm a*	*C*
2	*b*				$0\frac{1}{2}0$ *C*
2	*c*				$\frac{1}{2}0\frac{1}{2}$ *C*
2	*d*				$00\frac{1}{2}$ *C*
4	*e*	2..		*Cmmm g*	*C*2*x*
4	*f*				$00\frac{1}{2}$ *C*2*x*
4	*g*	.2.			*C*2*y*
4	*h*				$00\frac{1}{2}$ *C*2*y*
4	*i*	..2		*Cmmm k*	*C*2*z*
4	*j*				$0\frac{1}{2}0$ *C*2*z*
4	*k*	..2		*Cmme g*	$\frac{1}{4}\frac{1}{4}0$ 2.. $P_{ab}F1z$
8	*l*	1	*	*C*222 *l*	*C*2*x*2*yz*

22 *F*222

4	*a*	222		*Fmmm a*	*F*
4	*b*				$00\frac{1}{2}$ *F*
4	*c*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*				$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ *F*
8	*e*	2..		*Fmmm g*	*F*2*x*
8	*j*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*2*x*
8	*f*	.2.			*F*2*y*
8	*i*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*2*y*
8	*g*	..2			*F*2*z*
8	*h*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*2*z*
16	*k*	1	*	*F*222 *k*	*F*2*x*2*yz*

23 *I*222

2	*a*	222		*Immm a*	*I*
2	*b*				$\frac{1}{2}00$ *I*
2	*c*				$00\frac{1}{2}$ *I*
2	*d*				$0\frac{1}{2}0$ *I*
4	*e*	2..		*Immm e*	*I*2*x*
4	*f*				$00\frac{1}{2}$ *I*2*x*
4	*g*	.2.			*I*2*y*
4	*h*				$\frac{1}{2}00$ *I*2*y*
4	*i*	..2			*I*2*z*
4	*j*				$0\frac{1}{2}0$ *I*2*z*
8	*k*	1	*	*I*222 *k*	*I*2*x*2*yz*

24 $I2_12_12_1$

4	*a*	2..		*Imma e*	$\frac{1}{4}0\frac{1}{4}$ ..2 C_cB_b1x
4	*b*	.2.			$\frac{1}{4}\frac{1}{4}0$ 2.. A_aC_c1y
4	*c*	..2			$0\frac{1}{4}\frac{1}{4}$ .2. B_bA_a1z
8	*d*	1	*	$I2_12_12_1$ *d*	$\frac{1}{4}0\frac{1}{4}$ ..2 C_cB_b1x2yz

25 *Pmm*2

1	*a*	*mm*2		*Pmmm a*	*P*[*z*]
1	*b*				$0\frac{1}{2}0$ *P*[*z*]
1	*c*				$\frac{1}{2}00$ *P*[*z*]
1	*d*				$\frac{1}{2}\frac{1}{2}0$ *P*[*z*]
2	*e*	.*m*.		*Pmmm i*	*P*2*x*[*z*]
2	*f*				$0\frac{1}{2}0$ *P*2*x*[*z*]
2	*g*	*m*..			*P*2*y*[*z*]
2	*h*				$\frac{1}{2}00$ *P*2*y*[*z*]
4	*i*	1		*Pmmm u*	*P*2*x*2*y*[*z*]

26 $Pmc2_1$

2	*a*	*m*..		*Pmma e*	2.. P_cA1y[*z*]
2	*b*				$\frac{1}{2}00$ 2.. P_cA1y[*z*]
4	*c*	1		*Pmma k*	2.. P_cA1y2x[*z*]

27 *Pcc*2

2	*a*	..2		*Pmmm a*	P_c[*z*]
2	*b*				$0\frac{1}{2}0$ P_c[*z*]

Table 3.4.3.3 (continued)

2	*c*			$\frac{1}{2}00\ P_c[z]$
2	*d*			$\frac{1}{2}\frac{1}{2}0\ P_c[z]$
4	*e*	1	*Pccm q*	$2..\ P_c2xy[z]$

28 *Pma2*

2	*a*	..2	*Pmmm a*	$P_a[z]$
2	*b*			$0\frac{1}{2}0\ P_a[z]$
2	*c*	*m*..	*Pmma e*	$\frac{1}{4}00\ ..2\ P_aC1y[z]$
4	*d*	1	*Pmma i*	$m..\ P_a2xy[z]$

29 *Pca*2_1

4	*a*	1	*Pbcm d*	$.2\bar{1}\ P_{ac}B_aC_cF1xy[z]$

30 *Pnc2*

2	*a*	..2	*Cmmm a*	$A[z]$
2	*b*			$\frac{1}{2}00\ A[z]$
4	*c*	1	*Pmna h*	$2..\ A2xy[z]$

31 *Pmn*2_1

2	*a*	*m*..	*Pmmn a*	$..2_1\ BI1y[z]$
4	*b*	1	*Pmmn e*	$..2_1\ BI1y2x[z]$

32 *Pba2*

2	*a*	..2	*Cmmm a*	$C[z]$
2	*b*			$0\frac{1}{2}0\ C[z]$
4	*c*	1	*Pbam g*	$b..\ C2xy[z]$

33 *Pna*2_1

4	*a*	1	*Pnma c*	$\bar{1}2_1.\ C_cA_aFI_a1xy[z]$

34 *Pnn2*

2	*a*	..2	*Immm a*	$I[z]$
2	*b*			$0\frac{1}{2}0\ I[z]$
4	*c*	1	*Pnnm g*	$n..\ I2xy[z]$

35 *Cmm2*

2	*a*	*mm*2	*Cmmm a*	$C[z]$
2	*b*			$0\frac{1}{2}0\ C[z]$
4	*c*	..2	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_{ab}[z]$
4	*d*	.*m*.	*Cmmm g*	$C2x[z]$
4	*e*	*m*..		$C2y[z]$
8	*f*	1	*Cmmm p*	$C2x2y[z]$

36 *Cmc*2_1

4	*a*	*m*..	*Cmcm c*	$2_1..\ C_cF1y[z]$
8	*b*	1	*Cmcm g*	$2_1..\ C_cF1y2x[z]$

37 *Ccc2*

4	*a*	..2	*Cmmm a*	$C_c[z]$
4	*b*			$0\frac{1}{2}0\ C_c[z]$
4	*c*	..2	*Fmmm a*	$\frac{1}{4}\frac{1}{4}0\ F[z]$
8	*d*	1	*Cccm l*	$n..\ C_c2xy[z]$

38 *Amm2*

2	*a*	*mm*2	*Cmmm a*	$A[z]$
2	*b*			$\frac{1}{2}00\ A[z]$
4	*c*	.*m*.	*Cmmm k*	$A2x[z]$
4	*d*	*m*..	*Cmmm g*	$A2y[z]$
4	*e*			$\frac{1}{2}00\ A2y[z]$
8	*f*	1	*Cmmm n*	$A2x2y[z]$

39 *Aem2*

4	*a*	..2	*Pmmm a*	$P_{bc}[z]$
4	*b*			$\frac{1}{2}00\ P_{bc}[z]$
4	*c*	.*m*.	*Cmme g*	$0\frac{1}{4}0\ ..2\ P_{bc}F1x[z]$
8	*d*	1	*Cmme m*	$.m.\ P_{bc}2xy[z]$

40 *Ama2*

4	*a*	..2	*Cmmm a*	$A_a[z]$
4	*b*	*m*..	*Cmcm c*	$\frac{1}{4}00\ ..2_1\ A_aF1y[z]$
8	*c*	1	*Cmcm f*	$.n.\ A_a2xy[z]$

41 *Aea2*

4	*a*	..2	*Fmmm a*	$F[z]$
8	*b*	1	*Cmce f*	$.2.\ F2xy[z]$

42 *Fmm2*

4	*a*	*mm*2	*Fmmm a*	$F[z]$
8	*b*	..2	*Pmmm a*	$\frac{1}{4}\frac{1}{4}0\ P_2[z]$
8	*c*	*m*..	*Fmmm g*	$F2y[z]$
8	*d*	.*m*.		$F2x[z]$
16	*e*	1	*Fmmm m*	$F2x2y[z]$

43 *Fdd2*

8	*a*	..2	*Fddd a*	$D[z]$
16	*b*	1	* *Fdd2 b*	$d..\ D2xy[z]$

44 *Imm2*

2	*a*	*mm*2	*Immm a*	$I[z]$
2	*b*			$0\frac{1}{2}0\ I[z]$
4	*c*	.*m*.	*Immm e*	$I2x[z]$
4	*d*	*m*..		$I2y[z]$
8	*e*	1	*Immm l*	$I2x2y[z]$

45 *Iba2*

4	*a*	..2	*Cmmm a*	$C_c[z]$
4	*b*			$0\frac{1}{2}0\ C_c[z]$
8	*c*	1	*Ibam j*	$b..\ C_c2xy[z]$

46 *Ima2*

4	*a*	..2	*Cmmm a*	$A_a[z]$
4	*b*	*m*..	*Imma e*	$\frac{1}{4}00\ 2..\ A_aC_c1y[z]$
8	*c*	1	*Imma h*	$2..\ A_a2xy[z]$

47 *Pmmm*

1	*a*	*mmm*	* *Pmmm a*	P
1	*b*			$\frac{1}{2}00\ P$

Table 3.4.3.3 (continued)

1	*c*				$00\frac{1}{2}$ *P*
1	*d*				$\frac{1}{2}0\frac{1}{2}$ *P*
1	*e*				$0\frac{1}{2}0$ *P*
1	*f*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*g*				$0\frac{1}{2}\frac{1}{2}$ *P*
1	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$
2	*i*	2*mm*	*	*Pmmm i*	*P*2*x*
2	*j*				$00\frac{1}{2}$ *P*2*x*
2	*k*				$0\frac{1}{2}0$ *P*2*x*
2	*l*				$0\frac{1}{2}\frac{1}{2}$ *P*2*x*
2	*m*	*m*2*m*			*P*2*y*
2	*n*				$00\frac{1}{2}$ *P*2*y*
2	*o*				$\frac{1}{2}00$ *P*2*y*
2	*p*				$\frac{1}{2}0\frac{1}{2}$ *P*2*y*
2	*q*	*mm*2			*P*2*z*
2	*r*				$0\frac{1}{2}0$ *P*2*z*
2	*s*				$\frac{1}{2}00$ *P*2*z*
2	*t*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*u*	*m*..	*	*Pmmm u*	*P*2*y*2*z*
4	*v*				$\frac{1}{2}00$ *P*2*y*2*z*
4	*w*	*.m.*			*P*2*x*2*z*
4	*x*				$0\frac{1}{2}0$ *P*2*x*2*z*
4	*y*	*..m*			*P*2*x*2*y*
4	*z*				$00\frac{1}{2}$ *P*2*x*2*y*
8	α	1	*	*Pmmm* α	*P*2*x*2*y*2*z*

48 *Pnnn*

2	*a*	222		*Immm a*	*I*
2	*b*				$\frac{1}{2}00$ *I*
2	*c*				$00\frac{1}{2}$ *I*
2	*d*				$0\frac{1}{2}0$ *I*
4	*e*	$\bar{1}$		*Fmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*f*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
4	*g*	2..		*Immm e*	*I*2*x*
4	*h*				$00\frac{1}{2}$ *I*2*x*
4	*i*	.2.			*I*2*y*
4	*j*				$\frac{1}{2}00$ *I*2*y*
4	*k*	..2			*I*2*z*
4	*l*				$0\frac{1}{2}0$ *I*2*z*
8	*m*	1	*	*Pnnn m*	*n*.. *I*2*x*2*yz*

49 *Pccm*

2	*a*	..2/*m*		*Pmmm a*	P_c
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*				$0\frac{1}{2}0$ P_c
2	*d*				$\frac{1}{2}00$ P_c
2	*e*	222		*Pmmm a*	$00\frac{1}{4}$ P_c
2	*f*				$\frac{1}{2}0\frac{1}{4}$ P_c
2	*g*				$0\frac{1}{2}\frac{1}{4}$ P_c
2	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*i*	2..		*Pmmm i*	$00\frac{1}{4}$ P_c*2x*
4	*j*				$0\frac{1}{2}\frac{1}{4}$ P_c*2x*
4	*k*	.2.			$00\frac{1}{4}$ P_c*2y*
4	*l*				$\frac{1}{2}0\frac{1}{4}$ P_c*2y*
4	*m*	..2		*Pmmm i*	P_c*2z*
4	*n*				$\frac{1}{2}\frac{1}{2}0$ P_c*2z*
4	*o*				$0\frac{1}{2}0$ P_c*2z*
4	*p*				$\frac{1}{2}00$ P_c*2z*
4	*q*	*..m*	*	*Pccm q*	2.. P_c*2xy*
8	*r*	1	*	*Pccm r*	*c*.. P_c*2xy*2*z*

50 *Pban*

2	*a*	222		*Cmmm a*	*C*
2	*b*				$\frac{1}{2}00$ *C*
2	*c*				$\frac{1}{2}0\frac{1}{2}$ *C*
2	*d*				$00\frac{1}{2}$ *C*
4	*e*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	2..		*Cmmm g*	*C*2*x*
4	*h*				$00\frac{1}{2}$ *C*2*x*
4	*i*	.2.			*C*2*y*
4	*j*				$00\frac{1}{2}$ *C*2*y*
4	*k*	..2		*Cmmm k*	*C*2*z*
4	*l*				$0\frac{1}{2}0$ *C*2*z*
8	*m*	1	*	*Pban m*	*b*.. *C*2*x*2*yz*

51 *Pmma*

2	*a*	.2/*m*.		*Pmmm a*	P_a
2	*b*				$0\frac{1}{2}0$ P_a
2	*c*				$00\frac{1}{2}$ P_a
2	*d*				$0\frac{1}{2}\frac{1}{2}$ P_a
2	*e*	*mm*2	*	*Pmma e*	$\frac{1}{4}00$ .2. P_a*B*1*z*
2	*f*				$\frac{1}{4}\frac{1}{2}0$ .2. P_a*B*1*z*
4	*g*	.2.		*Pmmm i*	P_a*2y*
4	*h*				$00\frac{1}{2}$ P_a*2y*
4	*i*	*.m.*	*	*Pmma i*	*m*.. P_a*2xz*
4	*j*				$0\frac{1}{2}0$ *m*.. P_a*2xz*
4	*k*	*m*..	*	*Pmma k*	$\frac{1}{4}00$ .2. P_a*B*1*z*2*y*
8	*l*	1	*	*Pmma l*	*m*.. P_a*2xz*2*y*

52 *Pnna*

4	*a*	$\bar{1}$		*Cmmm a*	A_a
4	*b*				$00\frac{1}{2}$ A_a
4	*c*	..2		*Imma e*	$\frac{1}{4}0\frac{1}{4}$ .2. B_bA_a1*z*
4	*d*	2..		*Cmcm c*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ ..2_1 B_b*F*1*x*
8	*e*	1	*	*Pnna e*	2.2 A_a*2xyz*

53 *Pmna*

2	*a*	2/*m*..		*Cmmm a*	*B*
2	*b*				$\frac{1}{2}00$ *B*
2	*c*				$\frac{1}{2}\frac{1}{2}0$ *B*
2	*d*				$0\frac{1}{2}0$ *B*
4	*e*	2..		*Cmmm g*	*B*2*x*
4	*f*				$0\frac{1}{2}0$ *B*2*x*
4	*g*	.2.		*Pmma e*	$\frac{1}{4}0\frac{1}{4}$ (2.. P_c*A*1*y*)$_a$
4	*h*	*m*..	*	*Pmna h*	.2. *B*2*yz*
8	*i*	1	*	*Pmna i*	.2. *B*2*yz*2*x*

Table 3.4.3.3 (continued)

54 *Pcca*

4	*a*	$\bar{1}$		*Pmmm a*	P_{ac}
4	*b*				$0\frac{1}{2}0$ P_{ac}
4	*c*	.2.		*Cmme g*	$00\frac{1}{4}$ ..2 $P_{ac}F1y$
4	*d*	..2		*Pmma e*	$\frac{1}{4}00$ $(.2.\ P_aB1z)_c$
4	*e*				$\frac{1}{4}\frac{1}{2}0$ $(.2.\ P_aB1z)_c$
8	*f*	1	*	*Pcca f*	.22 $P_{ac}2xyz$

55 *Pbam*

2	*a*	..2/*m*		*Cmmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*				$0\frac{1}{2}0$ *C*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e*	..2		*Cmmm k*	*C*2*z*
4	*f*				$0\frac{1}{2}0$ *C*2*z*
4	*g*	..*m*	*	*Pbam g*	*b*.. *C*2*xy*
4	*h*				$00\frac{1}{2}$ *b*.. *C*2*xy*
8	*i*	1	*	*Pbam i*	*b*.. *C*2*xy*2*z*

56 *Pccn*

4	*a*	$\bar{1}$		*Fmmm a*	*F*
4	*b*				$00\frac{1}{2}$ *F*
4	*c*	..2		*Pmmn a*	$\frac{1}{4}\frac{1}{4}0$ $(2_1..\ CI1z)_c$
4	*d*				$\frac{1}{4}\frac{3}{4}0$ $(2_1..\ CI1z)_c$
8	*e*	1	*	*Pccn e*	*c*.2 *F*2*xyz*

57 *Pbcm*

4	*a*	$\bar{1}$		*Pmmm a*	P_{bc}
4	*b*				$\frac{1}{2}00$ P_{bc}
4	*c*	2..		*Pmma e*	$0\frac{1}{4}0$ $(..2\ P_bC1x)_c$
4	*d*	..*m*	*	*Pbcm d*	$00\frac{1}{4}$ $2.\bar{1}$ $P_{bc}A_bC_cF1xy$
8	*e*	1	*	*Pbcm e*	2.*m* $P_{bc}2xyz$

58 *Pnnm*

2	*a*	..2/*m*		*Immm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
2	*c*				$0\frac{1}{2}0$ *I*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *I*
4	*e*	..2		*Immm e*	*I*2*z*
4	*f*				$0\frac{1}{2}0$ *I*2*z*
4	*g*	..*m*	*	*Pnnm g*	*n*.. *I*2*xy*
8	*h*	1	*	*Pnnm h*	*n*.. *I*2*xy*2*z*

59 *Pmmn*

2	*a*	*mm*2	*	*Pmmn a*	$2_1..\ CI1z$
2	*b*				$0\frac{1}{2}0$ $2_1..\ CI1z$
4	*c*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*d*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*e*	*m*..	*	*Pmmn e*	$2_1..\ CI1z2y$
4	*f*	.*m*.			$.2_1.\ CI1z2x$
8	*g*	1	*	*Pmmn g*	$\frac{1}{4}\frac{1}{4}0$ *mm*. $P_{ab}2xyz$

60 *Pbcn*

4	*a*	$\bar{1}$		*Cmmm a*	C_c
4	*b*				$0\frac{1}{2}0$ C_c
4	*c*	.2.		*Cmcm c*	$00\frac{1}{4}$ $2_1..\ C_cF1y$
8	*d*	1	*	*Pbcn d*	*b*2. C_c2xyz

61 *Pbca*

4	*a*	$\bar{1}$		*Fmmm a*	*F*
4	*b*				$00\frac{1}{2}$ *F*
8	*c*	1	*	*Pbca c*	*bc*. *F*2*xyz*

62 *Pnma*

4	*a*	$\bar{1}$		*Cmmm a*	B_b
4	*b*				$00\frac{1}{2}$ B_b
4	*c*	.*m*.	*	*Pnma c*	$0\frac{1}{4}0$ $\bar{1}.2_1$ $B_bA_aFI_a1xz$
8	*d*	1	*	*Pnma d*	.*ma* B_b2xyz

63 *Cmcm*

4	*a*	2/*m*..		*Cmmm a*	C_c
4	*b*				$0\frac{1}{2}0$ C_c
4	*c*	*m*2*m*	*	*Cmcm c*	$00\frac{1}{4}$ $2_1..\ C_cF1y$
8	*d*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*e*	2..		*Cmmm g*	C_c2x
8	*f*	*m*..	*	*Cmcm f*	.*n*. C_c2yz
8	*g*	..*m*	*	*Cmcm g*	$00\frac{1}{4}$ $2_1..\ C_cF1y2x$
16	*h*	1	*	*Cmcm h*	.*n*. C_c2yz2x

64 *Cmce*

4	*a*	2/*m*..		*Fmmm a*	*F*
4	*b*				$00\frac{1}{2}$ *F*
8	*c*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*d*	2..		*Fmmm g*	*F*2*x*
8	*e*	.2.		*Pmma e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $(2..\ P_cA1y)_{ab}$
8	*f*	*m*..	*	*Cmce f*	.2. *F*2*yz*
16	*g*	1	*	*Cmce g*	.2. *F*2*yz*2*x*

65 *Cmmm*

2	*a*	*mmm*	*	*Cmmm a*	*C*
2	*b*				$\frac{1}{2}00$ *C*
2	*c*				$\frac{1}{2}0\frac{1}{2}$ *C*
2	*d*				$00\frac{1}{2}$ *C*
4	*e*	..2/*m*		*Pmmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	2*mm*	*	*Cmmm g*	*C*2*x*
4	*h*				$00\frac{1}{2}$ *C*2*x*
4	*i*	*m*2*m*			*C*2*y*
4	*j*				$00\frac{1}{2}$ *C*2*y*
4	*k*	*mm*2	*	*Cmmm k*	*C*2*z*
4	*l*				$0\frac{1}{2}0$ *C*2*z*
8	*m*	..2		*Pmmm i*	$\frac{1}{4}\frac{1}{4}0$ $P_{ab}2z$
8	*n*	*m*..	*	*Cmmm n*	*C*2*y*2*z*
8	*o*	.*m*.			*C*2*x*2*z*
8	*p*	..*m*	*	*Cmmm p*	*C*2*x*2*y*
8	*q*				$00\frac{1}{2}$ *C*2*x*2*y*
16	*r*	1	*	*Cmmm r*	*C*2*x*2*y*2*z*

Table 3.4.3.3 (continued)

66 *Cccm*

4	*a*	222		*Cmmm a*	$00\frac{1}{4}\ C_c$
4	*b*				$0\frac{1}{2}\frac{1}{4}\ C_c$
4	*c*	..2/*m*		*Cmmm a*	C_c
4	*d*				$0\frac{1}{2}0\ C_c$
4	*e*	..2/*m*		*Fmmm a*	$\frac{1}{4}\frac{1}{4}0\ F$
4	*f*				$\frac{1}{4}\frac{3}{4}0\ F$
8	*g*	2..		*Cmmm g*	$00\frac{1}{4}\ C_c2x$
8	*h*	.2.			$00\frac{1}{4}\ C_c2y$
8	*i*	..2		*Cmmm k*	C_c2z
8	*j*				$0\frac{1}{2}0\ C_c2z$
8	*k*	..2		*Fmmm g*	$\frac{1}{4}\frac{1}{4}0\ F2z$
8	*l*	..*m*	*	*Cccm l*	$c..\ C_c2xy$
16	*m*	1	*	*Cccm m*	$c..\ C_c2xy2z$

67 *Cmme*

4	*a*	222		*Pmmm a*	$\frac{1}{4}00\ P_{ab}$
4	*b*				$\frac{1}{4}0\frac{1}{2}\ P_{ab}$
4	*c*	2/*m*..		*Pmmm a*	P_{ab}
4	*d*				$00\frac{1}{2}\ P_{ab}$
4	*e*	.2/*m*.			$\frac{1}{4}\frac{1}{4}0\ P_{ab}$
4	*f*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}\ P_{ab}$
4	*g*	*mm*2	*	*Cmme g*	$0\frac{1}{4}0\ 2..\ P_{ab}F1z$
8	*h*	2..		*Pmmm i*	$P_{ab}2x$
8	*i*				$00\frac{1}{2}\ P_{ab}2x$
8	*j*	.2.			$\frac{1}{4}00\ P_{ab}2y$
8	*k*				$\frac{1}{4}0\frac{1}{2}\ P_{ab}2y$
8	*l*	..2		*Pmmm i*	$\frac{1}{4}00\ P_{ab}2z$
8	*m*	*m*..	*	*Cmme m*	$.m.\ P_{ab}2yz$
8	*n*	.*m*.			$0\frac{1}{4}0\ m..\ P_{ab}2xz$
16	*o*	1	*	*Cmme o*	$.m.\ P_{ab}2yz2x$

68 *Ccce*

4	*a*	222		*Fmmm a*	F
4	*b*				$00\frac{1}{2}\ F$
8	*c*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}0\frac{1}{4}\ P_2$
8	*d*				$0\frac{1}{4}\frac{1}{4}\ P_2$
8	*e*	2..		*Fmmm g*	$F2x$
8	*f*	.2.			$F2y$
8	*g*	..2		*Fmmm g*	$F2z$
8	*h*	..2		*Cmme g*	$\frac{1}{4}\frac{1}{4}0\ (2..\ P_{ab}F1z)_c$
16	*i*	1	*	*Ccce i*	$c..\ F2x2yz$

69 *Fmmm*

4	*a*	*mmm*	*	*Fmmm a*	F
4	*b*				$00\frac{1}{2}\ F$
8	*c*	2/*m*..		*Pmmm a*	$0\frac{1}{4}\frac{1}{4}\ P_2$
8	*d*	.2/*m*.			$\frac{1}{4}0\frac{1}{4}\ P_2$
8	*e*	..2/*m*			$\frac{1}{4}\frac{1}{4}0\ P_2$
8	*f*	222		*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*g*	2*mm*	*	*Fmmm g*	$F2x$
8	*h*	*m*2*m*			$F2y$
8	*i*	*mm*2			$F2z$
16	*j*	..2		*Pmmm i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2 2z$
16	*k*	.2.			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2 2y$
16	*l*	2..			$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2 2x$
16	*m*	*m*..	*	*Fmmm m*	$F2y2z$
16	*n*	.*m*.			$F2x2z$
16	*o*	..*m*			$F2x2y$
32	*p*	1	*	*Fmmm p*	$F2x2y2z$

70 *Fddd*

8	*a*	222	*	*Fddd a*	D
8	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ D$
16	*c*	$\bar{1}$	*	*Fddd c*	T
16	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ T$
16	*e*	2..	*	*Fddd e*	$D2x$
16	*f*	.2.			$D2y$
16	*g*	..2			$D2z$
32	*h*	1	*	*Fddd h*	$d..\ D2x2yz$

71 *Immm*

2	*a*	*mmm*	*	*Immm a*	I
2	*b*				$0\frac{1}{2}\frac{1}{2}\ I$
2	*c*				$\frac{1}{2}\frac{1}{2}0\ I$
2	*d*				$\frac{1}{2}0\frac{1}{2}\ I$
4	*e*	2*mm*	*	*Immm e*	$I2x$
4	*f*				$0\frac{1}{2}0\ I2x$
4	*g*	*m*2*m*			$I2y$
4	*h*				$00\frac{1}{2}\ I2y$
4	*i*	*mm*2			$I2z$
4	*j*				$\frac{1}{2}00\ I2z$
8	*k*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*l*	*m*..	*	*Immm l*	$I2y2z$
8	*m*	.*m*.			$I2x2z$
8	*n*	..*m*			$I2x2y$
16	*o*	1	*	*Immm o*	$I2x2y2z$

72 *Ibam*

4	*a*	222		*Cmmm a*	$00\frac{1}{4}\ C_c$
4	*b*				$\frac{1}{2}0\frac{1}{4}\ C_c$
4	*c*	..2/*m*		*Cmmm a*	C_c
4	*d*				$\frac{1}{2}00\ C_c$
8	*e*	$\bar{1}$		*Pmmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*f*	2..		*Cmmm g*	$00\frac{1}{4}\ C_c2x$
8	*g*	.2.			$00\frac{1}{4}\ C_c2y$
8	*h*	..2		*Cmmm k*	C_c2z
8	*i*				$0\frac{1}{2}0\ C_c2z$
8	*j*	..*m*	*	*Ibam j*	$c..\ C_c2xy$
16	*k*	1	*	*Ibam k*	$c..\ C_c2xy2z$

73 *Ibca*

8	*a*	$\bar{1}$		*Pmmm a*	P_2
8	*b*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*c*	2..		*Cmme g*	$00\frac{1}{4}\ (.2.\ P_{bc}F1x)_a$
8	*d*	.2.			$\frac{1}{4}00\ (..2\ P_{ac}F1y)_b$
8	*e*	..2			$0\frac{1}{4}0\ (2..\ P_{ab}F1z)_c$
16	*f*	1	*	*Ibca f*	$22.\ P_2 2xyz$

Table 3.4.3.3 (continued)

74 *Imma*

4	*a*	2/*m*..		*Cmmm a*	B_b
4	*b*				$00\frac{1}{2}$ B_b
4	*c*	.2/*m*.			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ A_a
4	*d*				$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ A_a
4	*e*	*mm*2	*	*Imma e*	$0\frac{1}{4}0$ .2. B_bA_a1z
8	*f*	2..		*Cmmm g*	B_b2x
8	*g*	.2.			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ A_a2y
8	*h*	*m*..	*	*Imma h*	.2. B_b2yz
8	*i*	.*m*.			$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 2.. A_a2xz
16	*j*	1	*	*Imma j*	.2. B_b2yz2x

75 *P*4

1	*a*	4..		*P*4/*mmm a*	*P*[*z*]
1	*b*				$\frac{1}{2}\frac{1}{2}0$ *P*[*z*]
2	*c*	2..		*P*4/*mmm a*	$0\frac{1}{2}0$ *C*[*z*]
4	*d*	1		*P*4/*m j*	*P*4*xy*[*z*]

76 $P4_1$

4	*a*	1	*	$P4_3$ *a*	4_1.. $P_{cc}{}^{v}DI_c1xy[z]$

77 $P4_2$

2	*a*	2..		*P*4/*mmm a*	$P_c[z]$
2	*b*				$\frac{1}{2}\frac{1}{2}0$ $P_c[z]$
2	*c*	2..		*I*4/*mmm a*	$0\frac{1}{2}0$ *I*[*z*]
4	*d*	1		$P4_2/m$ *j*	$\bar{4}$.. $P_c2xy[z]$

78 $P4_3$

4	*a*		*	$P4_3$ *a*	4_3.. $P_{cc}{}^{v}DI_c1xy[z]$

79 *I*4

2	*a*	4..		*I*4/*mmm a*	*I*[*z*]
4	*b*	2..		*P*4/*mmm a*	$0\frac{1}{2}0$ $C_c[z]$
8	*c*	1		*I*4/*m h*	*I*4*xy*[*z*]

80 $I4_1$

4	*a*	2..		$I4_1/amd$ *a*	${}^{v}D[z]$
8	*b*	1	*	$I4_1$ *b*	4_1.. ${}^{v}D2xy[z]$

81 $P\bar{4}$

1	*a*	$\bar{4}$..		*P*4/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
1	*c*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	2..		*P*4/*mmm g*	*P*2*z*
2	*f*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
2	*g*	2..		*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*h*	1	*	$P\bar{4}$ *h*	*P*4*xyz*

82 $I\bar{4}$

2	*a*	$\bar{4}$..		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
2	*c*				$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*				$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2..		*I*4/*mmm e*	*I*2*z*
4	*f*				$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*g*	1	*	$I\bar{4}$ *g*	*I*4*xyz*

83 *P*4/*m*

1	*a*	4/*m*..		*P*4/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
1	*c*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	2/*m*..		*P*4/*mmm a*	$0\frac{1}{2}0$ *C*
2	*f*				$0\frac{1}{2}\frac{1}{2}$ *C*
2	*g*	4..		*P*4/*mmm g*	*P*2*z*
2	*h*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*j*	*m*..	*	*P*4/*m j*	*P*4*xy*
4	*k*				$00\frac{1}{2}$ *P*4*xy*
8	*l*	1	*	*P*4/*m l*	*P*4*xy*2*z*

84 $P4_2/m$

2	*a*	2/*m*..		*P*4/*mmm a*	P_c
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	2/*m*..		*I*4/*mmm a*	$0\frac{1}{2}0$ *I*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *I*
2	*e*	$\bar{4}$..		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*f*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*g*	2..		*P*4/*mmm g*	P_c2z
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2..		*I*4/*mmm e*	$0\frac{1}{2}0$ *I*2*z*
4	*j*	*m*..	*	$P4_2/m$ *j*	$\bar{4}$.. P_c2xy
8	*k*	1	*	$P4_2/m$ *k*	$\bar{4}$.. P_c2xy2z

85 *P*4/*n*

2	*a*	$\bar{4}$..		*P*4/*mmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*	4..		*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*d*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*e*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*f*	2..		*P*4/*mmm g*	*C*2*z*
8	*g*	1	*	*P*4/*n g*	$\bar{1}$ *C*4*xyz*

86 $P4_2/n$

2	*a*	$\bar{4}$..		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	$\bar{1}$		*I*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*				$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ *F*
4	*e*	2..		*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
4	*f*	2..		*I*4/*mmm e*	*I*2*z*
8	*g*	1	*	$P4_2/n$ *g*	*n*.. *I*4*xyz*

87 *I*4/*m*

2	*a*	4/*m*..		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	2/*m*..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c

Table 3.4.3.3 (continued)

4	*e*	4..		*I*4/*mmm e*	*I*2*z*
8	*f*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*h*	*m*..	*	*I*4/*m h*	*I*4*xy*
16	*i*	1	*	*I*4/*m i*	*I*4*xy*2*z*

88 $I4_1/a$

4	*a*	$\bar{4}$..		$I4_1/amd$ *a*	^{v}D
4	*b*				$00\frac{1}{2}$ ^{v}D
8	*c*	$\bar{1}$		$I4_1/amd$ *c*	^{v}T
8	*d*				$00\frac{1}{2}$ ^{v}T
8	*e*	2..		$I4_1/amd$ *e*	$^{v}D2z$
16	*f*	1	*	$I4_1/a$ *f*	*a*.. $^{v}D4xyz$

89 *P*422

1	*a*	422		*P*4/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
1	*c*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	222.		*P*4/*mmm a*	$\frac{1}{2}00$ *C*
2	*f*				$\frac{1}{2}0\frac{1}{2}$ *C*
2	*g*	4..		*P*4/*mmm g*	*P*2*z*
2	*h*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*j*	..2		*P*4/*mmm j*	*P*4*xx*
4	*k*				$00\frac{1}{2}$ *P*4*xx*
4	*l*	.2.		*P*4/*mmm l*	*P*4*x*
4	*m*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*4*x*
4	*n*				$00\frac{1}{2}$ *P*4*x*
4	*o*				$\frac{1}{2}\frac{1}{2}0$ *P*4*x*
8	*p*	1	*	*P*422 *p*	*P*4*x*2*yz*

90 $P42_12$

2	*a*	2.22		*P*4/*mmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*	4..		*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*d*	2..		*P*4/*mmm g*	*C*2*z*
4	*e*	..2		*P*4/*mbm g*	*.b. C*2*xx*
4	*f*				$00\frac{1}{2}$ *.b. C*2*xx*
8	*g*	1	*	$P42_12$ *g*	$.2_1$. *C*2*xx*2*yz*

91 $P4_122$

4	*a*	.2.	*	$P4_322$ *a*	$00\frac{3}{4}$ $4_1..$ $P_{cc}I_c1x$
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{3}{4}$ $4_1..$ $P_{cc}I_c1x$
4	*c*	..2	*	$P4_322$ *c*	$00\frac{3}{8}$ $4_1..$ $P_{cc}{}^{v}D1xx$
8	*d*	1	*	$P4_322$ *d*	$00\frac{3}{4}$ $4_1..$ $P_{cc}I_c1x2yz$

92 $P4_12_12$

4	*a*	..2	*	$P4_32_12$ *a*	$4_1..$ $I_c{}^{v}D1xx$
8	*b*	1	*	$P4_32_12$ *b*	$4_1..$ $I_c{}^{v}D1xx2yz$

93 $P4_222$

2	*a*	222.		*P*4/*mmm a*	P_c
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	222.		*I*4/*mmm a*	$0\frac{1}{2}0$ *I*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *I*
2	*e*	2.22		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*f*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*g*	2..		*P*4/*mmm g*	P_c2z
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2..		*I*4/*mmm e*	$0\frac{1}{2}0$ *I*2*z*
4	*j*	.2.		$P4_2/mmc$ *j*	..2 P_c2x
4	*k*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ..2 P_c2x
4	*l*				$00\frac{1}{2}$ ..2 P_c2x
4	*m*				$\frac{1}{2}\frac{1}{2}0$ ..2 P_c2x
4	*n*	..2		$P4_2/mcm$ *i*	$00\frac{1}{4}$ .2. P_c2xx
4	*o*				$00\frac{3}{4}$ .2. P_c2xx
8	*p*	1	*	$P4_222$ *p*	..2 P_c2x2yz

94 $P4_22_12$

2	*a*	2.22		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	2..		*I*4/*mmm e*	*I*2*z*
4	*d*	2..		*P*4/*nmm c*	$0\frac{1}{2}0$ $(..2\ CI1z)_c$
4	*e*	..2		$P4_2/mnm$ *f*	*.n. I*2*xx*
4	*f*				$00\frac{1}{2}$ *.n. I*2*xx*
8	*g*	1	*	$P4_22_12$ *g*	$.2_1$. *I*2*xx*2*yz*

95 $P4_322$

4	*a*	.2.	*	$P4_322$ *a*	$00\frac{1}{4}$ $4_3..$ $P_{cc}I_c1x$
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ $4_3..$ $P_{cc}I_c1x$
4	*c*	..2	*	$P4_322$ *c*	$00\frac{5}{8}$ $4_3..$ $P_{cc}{}^{v}D1xx$
8	*d*	1	*	$P4_322$ *d*	$00\frac{1}{4}$ $4_3..$ $P_{cc}I_c1x2yz$

96 $P4_32_12$

4	*a*	..2	*	$P4_32_12$ *a*	$4_3..$ $I_c{}^{v}D1xx$
8	*b*	1	*	$P4_32_12$ *b*	$4_3..$ $I_c{}^{v}D1xx2yz$

97 *I*422

2	*a*	422		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	222.		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	4..		*I*4/*mmm e*	*I*2*z*
8	*f*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*g*	..2		*I*4/*mmm h*	*I*4*xx*
8	*h*	.2.		*I*4/*mmm i*	*I*4*x*
8	*i*				$00\frac{1}{2}$ *I*4*x*
8	*j*	..2		*I*4/*mcm h*	$0\frac{1}{2}\frac{1}{4}$ *.b.* C_c2xx
16	*k*	1	*	*I*422 *k*	*I*4*x*2*yz*

98 $I4_122$

4	*a*	2.22		$I4_1/amd$ *a*	^{v}D
4	*b*				$00\frac{1}{2}$ ^{v}D
8	*c*	2..		$I4_1/amd$ *e*	$^{v}D2z$
8	*d*	..2	*	$I4_122$ *d*	.2. $^{v}D2xx$
8	*e*				.2. $^{v}D2x\bar{x}$

Table 3.4.3.3 (continued)

8	*f*	.2.	*	$I4_122$ *f*	..22 $^{v}TC_{cc}1x$
16	*g*	1	*	$I4_122$ *g*	.2. $^{v}D2xx2yz$

99 *P4mm*

1	*a*	4*mm*		*P*4/*mmm a*	*P*[*z*]
1	*b*				$\frac{1}{2}\frac{1}{2}0$ *P*[*z*]
2	*c*	2*mm*.		*P*4/*mmm a*	$\frac{1}{2}00$ *C*[*z*]
4	*d*	..*m*		*P*4/*mmm j*	*P*4*xx*[*z*]
4	*e*	.*m*.		*P*4/*mmm l*	*P*4*x*[*z*]
4	*f*				$\frac{1}{2}\frac{1}{2}0$ *P*4*x*[*z*]
8	*g*	1		*P*4/*mmm p*	*P*4*x*2*y*[*z*]

100 *P4bm*

2	*a*	4..		*P*4/*mmm a*	*C*[*z*]
2	*b*	2.*mm*		*P*4/*mmm a*	$\frac{1}{2}00$ *C*[*z*]
4	*c*	..*m*		*P*4/*mbm g*	$0\frac{1}{2}0$.*b*. *C*2*xx*[*z*]
8	*d*	1		*P*4/*mbm i*	..*m* *C*4*xy*[*z*]

101 $P4_2cm$

2	*a*	2.*mm*		*P*4/*mmm a*	P_c[*z*]
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c[*z*]
4	*c*	2..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c[*z*]
4	*d*	..*m*		$P4_2$/*mcm i*	.2. P_c2xx[*z*]
8	*e*	1		$P4_2$/*mcm n*	.2. P_c2xx2y[*z*]

102 $P4_2nm$

2	*a*	2.*mm*		*I*4/*mmm a*	*I*[*z*]
4	*b*	2..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c[*z*]
4	*c*	..*m*		$P4_2$/*mnm f*	.*n*. *I*2*xx*[*z*]
8	*d*	1		$P4_2$/*mnm i*	.*n*. *I*2*xx*2*y*[*z*]

103 *P4cc*

2	*a*	4..		*P*4/*mmm a*	P_c[*z*]
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c[*z*]
4	*c*	2..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c[*z*]
8	*d*	1		*P*4/*mcc m*	.*c*. P_c4*xy*[*z*]

104 *P4nc*

2	*a*	4..		*I*4/*mmm a*	*I*[*z*]
4	*b*	2..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c[*z*]
8	*c*	1		*P*4/*mnc h*	..2 *I*4*xy*[*z*]

105 $P4_2mc$

2	*a*	2*mm*.		*P*4/*mmm a*	P_c[*z*]
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c[*z*]
2	*c*	2*mm*.		*I*4/*mmm a*	$0\frac{1}{2}0$ *I*[*z*]
4	*d*	.*m*.		$P4_2$/*mmc j*	..2 P_c2x[*z*]
4	*e*				$\frac{1}{2}\frac{1}{2}0$ ..2 P_c2x[*z*]
8	*f*	1		$P4_2$/*mmc q*	..2 P_c2x2y[*z*]

106 $P4_2bc$

4	*a*	2..		*P*4/*mmm a*	C_c[*z*]
4	*b*	2..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c[*z*]
8	*c*	1		$P4_2$/*mbc h*	.*b*2 C_c2xy[*z*]

107 *I4mm*

2	*a*	4*mm*		*I*4/*mmm a*	*I*[*z*]
4	*b*	2*mm*.		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c[*z*]
8	*c*	..*m*		*I*4/*mmm h*	*I*4*xx*[*z*]
8	*d*	.*m*.		*I*4/*mmm i*	*I*4*x*[*z*]
16	*e*	1		*I*4/*mmm l*	*I*4*x*2*y*[*z*]

108 *I4cm*

4	*a*	4..		*P*4/*mmm a*	C_c[*z*]
4	*b*	2.*mm*		*P*4/*mmm a*	$\frac{1}{2}00$ C_c[*z*]
8	*c*	..*m*		*I*4/*mcm h*	$\frac{1}{2}00$.*b*. C_c2xx[*z*]
16	*d*	1		*I*4/*mcm k*	..*m* C_c4xy[*z*]

109 $I4_1md$

4	*a*	2*mm*.		$I4_1$/*amd a*	^{v}D[*z*]
8	*b*	.*m*.	*	$I4_1md$ *b*	..*d* $^{v}D2x$[*z*]
16	*c*	1	*	$I4_1md$ *c*	..*d* $^{v}D2x2y$[*z*]

110 $I4_1cd$

8	*a*	2..		*I*4/*mmm a*	F_c[*z*]
16	*b*	1	*	$I4_1cd$ *b*	.*bd* F_c2xy[*z*]

111 $P\bar{4}2m$

1	*a*	$\bar{4}2m$		*P*4/*mmm a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
1	*c*				$00\frac{1}{2}$ *P*
1	*d*				$\frac{1}{2}\frac{1}{2}0$ *P*
2	*e*	222.		*P*4/*mmm a*	$\frac{1}{2}00$ *C*
2	*f*				$\frac{1}{2}0\frac{1}{2}$ *C*
2	*g*	2.*mm*		*P*4/*mmm g*	*P*2*z*
2	*h*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	.2.		*P*4/*mmm l*	*P*4*x*
4	*j*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*4*x*
4	*k*				$00\frac{1}{2}$ *P*4*x*
4	*l*				$\frac{1}{2}\frac{1}{2}0$ *P*4*x*
4	*m*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*n*	..*m*	*	$P\bar{4}2m$ *n*	*P*4*xxz*
8	*o*	1	*	$P\bar{4}2m$ *o*	*P*4*xxz*2*y*

112 $P\bar{4}2c$

2	*a*	222.		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*c*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*b*	222.		*I*4/*mmm a*	$\frac{1}{2}0\frac{1}{4}$ *I*
2	*d*				$0\frac{1}{2}\frac{1}{4}$ *I*
2	*e*	$\bar{4}$..		*P*4/*mmm a*	P_c
2	*f*				$\frac{1}{2}\frac{1}{2}0$ P_c
4	*g*	.2.		$P4_2$/*mmc j*	$00\frac{1}{4}$ ..2 P_c2x
4	*h*				$\frac{1}{2}\frac{1}{2}\frac{3}{4}$ ..2 P_c2x
4	*i*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ ..2 P_c2x
4	*j*				$00\frac{3}{4}$ ..2 P_c2x
4	*k*	2..		*P*4/*mmm g*	P_c2z
4	*l*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*m*	2..		*I*4/*mmm e*	$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*n*	1	*	$P\bar{4}2c$ *n*	.2. P_c4xyz

Table 3.4.3.3 (continued)

113 $P\bar{4}2_1m$

2	*a*	$\bar{4}$..		*P*4/*mmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*	2.*mm*		*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*d*	2..		*P*4/*mmm g*	*C*2*z*
4	*e*	..*m*	*	$P\bar{4}2_1m$ *e*	$0\frac{1}{2}0$ .2_1. *CI*1*z*2*xx*
8	*f*	1	*	$P\bar{4}2_1m$ *f*	..*m* *C*4*xyz*

114 $P\bar{4}2_1c$

2	*a*	$\bar{4}$..		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	2..		*I*4/*mmm e*	*I*2*z*
4	*d*	2..		*P*4/*nmm c*	$0\frac{1}{2}0$ (..2 *CI*1*z*)$_c$
8	*e*	1	*	$P\bar{4}2_1c$ *e*	..*c* *I*4*xyz*

115 $P\bar{4}m2$

1	*a*	$\bar{4}m2$		*P*4/*mmm a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*c*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
1	*d*				$00\frac{1}{2}$ *P*
2	*e*	2*mm*.		*P*4/*mmm g*	*P*2*z*
2	*f*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
2	*g*	2*mm*.		*P*4/*nmm c*	$0\frac{1}{2}0$ ..2 *CI*1*z*
4	*h*	..2		*P*4/*mmm j*	*P*4*xx*
4	*i*				$00\frac{1}{2}$ *P*4*xx*
4	*j*	.*m*.	*	$P\bar{4}m2$ *j*	*P*4*xz*
4	*k*				$\frac{1}{2}\frac{1}{2}0$ *P*4*xz*
8	*l*	1	*	$P\bar{4}m2$ *l*	*P*4*xz*2*y*

116 $P\bar{4}c2$

2	*a*	2.22		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*c*	$\bar{4}$..		*P*4/*mmm a*	P_c
2	*d*				$\frac{1}{2}\frac{1}{2}0$ P_c
4	*e*	..2		*P*4$_2$/*mcm i*	$00\frac{1}{4}$ .2. P_c2*xx*
4	*f*				$00\frac{3}{4}$ .2. P_c2*xx*
4	*g*	2..		*P*4/*mmm g*	P_c2*z*
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2*z*
4	*i*	2..		*P*4/*nmm c*	$0\frac{1}{2}0$ (..2 *CI*1*z*)$_c$
8	*j*	1	*	$P\bar{4}c2$ *j*	..2 P_c4*xyz*

117 $P\bar{4}b2$

2	*a*	$\bar{4}$..		*P*4/*mmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*	2.22		*P*4/*mmm a*	$0\frac{1}{2}0$ *C*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e*	2..		*P*4/*mmm g*	*C*2*z*
4	*f*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*g*	..2		*P*4/*mbm g*	$0\frac{1}{2}0$.*b*. *C*2*xx*
4	*h*				$0\frac{1}{2}\frac{1}{2}$.*b*. *C*2*xx*
8	*i*	1	*	$P\bar{4}b2$ *i*	..2 *C*4*xyz*

118 $P\bar{4}n2$

2	*a*	$\bar{4}$..		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
2	*c*	2.22		*I*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*				$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2..		*I*4/*mmm e*	*I*2*z*
4	*f*	..2		*P*4$_2$/*mnm f*	$\frac{1}{2}0\frac{3}{4}$.*n*. *I*2*xx*
4	*g*				$0\frac{1}{2}\frac{1}{4}$.*n*. *I*2*xx*
4	*h*	2..		*I*4/*mmm e*	$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*i*	1	*	$P\bar{4}n2$ *i*	..2 *I*4*xyz*

119 $I\bar{4}m2$

2	*a*	$\bar{4}m2$		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
2	*c*				$0\frac{1}{2}\frac{1}{4}$ *I*
2	*d*				$0\frac{1}{2}\frac{3}{4}$ *I*
4	*e*	2*mm*.		*I*4/*mmm e*	*I*2*z*
4	*f*				$0\frac{1}{2}\frac{1}{4}$ *I*2*z*
8	*g*	..2		*I*4/*mmm h*	*I*4*xx*
8	*h*				$0\frac{1}{2}\frac{1}{4}$ *I*4*xx*
8	*i*	.*m*.	*	$I\bar{4}m2$ *i*	*I*4*xz*
16	*j*	1	*	$I\bar{4}m2$ *j*	*I*4*xz*2*y*

120 $I\bar{4}c2$

4	*a*	2.22		*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*d*				$0\frac{1}{2}0$ C_c
4	*b*	$\bar{4}$..		*P*4/*mmm a*	C_c
4	*c*				$0\frac{1}{2}\frac{1}{4}$ C_c
8	*e*	..2		*I*4/*mcm h*	$00\frac{1}{4}$.*b*. C_c2*xx*
8	*h*				$0\frac{1}{2}0$.*b*. C_c2*xx*
8	*f*	2..		*P*4/*mmm g*	C_c2*z*
8	*g*				$0\frac{1}{2}0$ C_c2*z*
16	*i*	1	*	$I\bar{4}c2$ *i*	..2 C_c4*xyz*

121 $I\bar{4}2m$

2	*a*	$\bar{4}2m$		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	222.		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	2.*mm*		*I*4/*mmm e*	*I*2*z*
8	*f*	.2.		*I*4/*mmm i*	*I*4*x*
8	*g*				$00\frac{1}{2}$ *I*4*x*
8	*h*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2*z*
8	*i*	..*m*	*	$I\bar{4}2m$ *i*	*I*4*xxz*
16	*j*	1	*	$I\bar{4}2m$ *j*	*I*4*xxz*2*y*

122 $I\bar{4}2d$

4	*a*	$\bar{4}$..		*I*4$_1$/*amd a*	^{v}D
4	*b*				$00\frac{1}{2}$ ^{v}D
8	*c*	2..		*I*4$_1$/*amd e*	^{v}D2*z*
8	*d*	.2.	*	$I\bar{4}2d$ *d*	$\bar{4}$.. $^{v}TF_c$1*x*
16	*e*	1	*	$I\bar{4}2d$ *e*	.2. ^{v}D4*xyz*

Table 3.4.3.3 (continued)

123 *P*4/*mmm*

1	*a*	4/*mmm*	*	*P*4/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
1	*c*				$\frac{1}{2}\frac{1}{2}0$ *P*
1	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*e*	*mmm.*		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{2}$ *C*
2	*f*				$0\frac{1}{2}0$ *C*
2	*g*	4*mm*	*	*P*4/*mmm g*	*P*2*z*
2	*h*				$\frac{1}{2}\frac{1}{2}0$ *P*2*z*
4	*i*	2*mm.*		*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*j*	*m*.2*m*	*	*P*4/*mmm j*	*P*4*xx*
4	*k*				$00\frac{1}{2}$ *P*4*xx*
4	*l*	*m*2*m.*	*	*P*4/*mmm l*	*P*4*x*
4	*m*				$00\frac{1}{2}$ *P*4*x*
4	*n*				$\frac{1}{2}\frac{1}{2}0$ *P*4*x*
4	*o*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*4*x*
8	*p*	*m..*	*	*P*4/*mmm p*	*P*4*x*2*y*
8	*q*				$00\frac{1}{2}$ *P*4*x*2*y*
8	*r*	*..m*	*	*P*4/*mmm r*	*P*4*xx*2*z*
8	*s*	*.m.*	*	*P*4/*mmm s*	*P*4*x*2*z*
8	*t*				$\frac{1}{2}\frac{1}{2}0$ *P*4*x*2*z*
16	*u*	1	*	*P*4/*mmm u*	*P*4*x*2*y*2*z*

124 *P*4/*mcc*

2	*a*	422		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*c*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
2	*b*	4/*m..*		*P*4/*mmm a*	P_c
2	*d*				$\frac{1}{2}\frac{1}{2}0$ P_c
4	*e*	2/*m..*		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*f*	222.		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*g*	4..		*P*4/*mmm g*	P_c2*z*
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2*z*
8	*i*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2*z*
8	*j*	..2		*P*4/*mmm j*	$00\frac{1}{4}$ P_c4*xx*
8	*k*	.2.		*P*4/*mmm l*	$00\frac{1}{4}$ P_c4*x*
8	*l*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c4*x*
8	*m*	*m..*	*	*P*4/*mcc m*	*.c.* P_c4*xy*
16	*n*	1	*	*P*4/*mcc n*	*.c.* P_c4*xy*2*z*

125 *P*4/*nbm*

2	*a*	422		*P*4/*mmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*	$\bar{4}$2*m*		*P*4/*mmm a*	$0\frac{1}{2}0$ *C*
2	*d*				$0\frac{1}{2}\frac{1}{2}$ *C*
4	*e*	*..*2/*m*		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*f*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*g*	4..		*P*4/*mmm g*	*C*2*z*
4	*h*	2.*mm*		*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
8	*i*	*..*2		*P*4/*mmm l*	*C*4*xx*
8	*j*				$00\frac{1}{2}$ *C*4*xx*
8	*k*	.2.		*P*4/*mmm j*	*C*4*x*
8	*l*				$00\frac{1}{2}$ *C*4*x*
8	*m*	*..m*	*	*P*4/*nbm m*	$0\frac{1}{2}0$ *..*2 *C*4*xxz*
16	*n*	1	*	*P*4/*nbm n*	*..m C*4*x*2*yz*

126 *P*4/*nnc*

2	*a*	422		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	222.		*P*4/*mmm a*	$\frac{1}{2}00$ C_c
4	*d*	$\bar{4}$..		*P*4/*mmm a*	$\frac{1}{2}0\frac{1}{4}$ C_c
4	*e*	4..		*I*4/*mmm e*	*I*2*z*
8	*f*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*g*	2..		*P*4/*mmm g*	$\frac{1}{2}00$ C_c2*z*
8	*h*	*..*2		*I*4/*mmm h*	*I*4*xx*
8	*i*	.2.		*I*4/*mmm i*	*I*4*x*
8	*j*				$00\frac{1}{2}$ *I*4*x*
16	*k*	1	*	*P*4/*nnc k*	*..c I*4*x*2*yz*

127 *P*4/*mbm*

2	*a*	4/*m..*		*P*4/*mmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*	*m.mm*		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{2}$ *C*
2	*d*				$0\frac{1}{2}0$ *C*
4	*e*	4..		*P*4/*mmm g*	*C*2*z*
4	*f*	2.*mm*		*P*4/*mmm g*	$0\frac{1}{2}0$ *C*2*z*
4	*g*	*m*.2*m*	*	*P*4/*mbm g*	$0\frac{1}{2}0$ *.b. C*2*xx*
4	*h*				$0\frac{1}{2}\frac{1}{2}$ *.b. C*2*xx*
8	*i*	*m..*	*	*P*4/*mbm i*	*..m C*4*xy*
8	*j*				$00\frac{1}{2}$ *..m C*4*xy*
8	*k*	*..m*	*	*P*4/*mbm k*	$0\frac{1}{2}0$ *.b. C*2*xx*2*z*
16	*l*	1	*	*P*4/*mbm l*	*..m C*4*xy*2*z*

128 *P*4/*mnc*

2	*a*	4/*m..*		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	2/*m..*		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	4..		*I*4/*mmm e*	*I*2*z*
8	*f*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2*z*
8	*g*	*..*2		*P*4/*mbm g*	$0\frac{1}{2}\frac{1}{4}$ $(.b.\ C2xx)_c$
8	*h*	*m..*	*	*P*4/*mnc h*	*..*2 *I*4*xy*
16	*i*	1	*	*P*4/*mnc i*	*..*2 *I*4*xy*2*z*

129 *P*4/*nmm*

2	*a*	$\bar{4}$*m*2		*P*4/*mmm a*	*C*
2	*b*				$00\frac{1}{2}$ *C*
2	*c*	4*mm*	*	*P*4/*nmm c*	$0\frac{1}{2}0$ *..*2 *CI*1*z*
4	*d*	*..*2/*m*		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}0$ P_{ab}
4	*e*				$\frac{1}{4}\frac{1}{4}\frac{1}{2}$ P_{ab}
4	*f*	2*mm.*		*P*4/*mmm g*	*C*2*z*
8	*g*	*..*2		*P*4/*mmm l*	*C*4*xx*
8	*h*				$00\frac{1}{2}$ *C*4*xx*
8	*i*	*.m.*	*	*P*4/*nmm i*	*..m C*4*xz*
8	*j*	*..m*	*	*P*4/*nmm j*	$0\frac{1}{2}0$ *..*2 *CI*1*z*4*xx*
16	*k*	1	*	*P*4/*nmm k*	*..m C*4*xz*2*y*

130 *P*4/*ncc*

4	*a*	2.22		*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*b*	$\bar{4}$..		*P*4/*mmm a*	C_c

Table 3.4.3.3 (continued)

4	*c*	4..		*P*4/*nmm c*	$0\frac{1}{2}0$ (..2 *CI*1*z*)$_c$
8	*d*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}0$ P_2
8	*e*	2..		*P*4/*mmm g*	C_c2z
8	*f*	..2		*I*4/*mcm h*	$00\frac{1}{4}$.*b*. C_c2xx
16	*g*	1	*	*P*4/*ncc g*	..*c*2 C_c4xyz

131 $P4_2/mmc$

2	*a*	*mmm*.		*P*4/*mmm a*	P_c
2	*b*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*c*	*mmm*.		*I*4/*mmm a*	$0\frac{1}{2}0$ I
2	*d*				$0\frac{1}{2}\frac{1}{2}$ I
2	*e*	$\bar{4}m2$		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*f*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*g*	2*mm*.		*P*4/*mmm g*	P_c2z
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	2*mm*.		*I*4/*mmm e*	$0\frac{1}{2}0$ *I*2*z*
4	*j*	*m*2*m*.	*	$P4_2/mmc$ *j*	..2 P_c2x
4	*k*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ..2 P_c2x
4	*l*				$00\frac{1}{2}$ ..2 P_c2x
4	*m*				$\frac{1}{2}\frac{1}{2}0$ ..2 P_c2x
8	*n*	..2		*P*4/*mmm j*	$00\frac{1}{4}$ P_c4xx
8	*o*	.*m*.	*	$P4_2/mmc$ *o*	..*c* P_c2x2z
8	*p*				$\frac{1}{2}\frac{1}{2}0$ ..*c* P_c2x2z
8	*q*	*m*..	*	$P4_2/mmc$ *q*	..2 P_c2x2y
16	*r*	1	*	$P4_2/mmc$ *r*	..*c* $P_c2x2y2z$

132 $P4_2/mcm$

2	*a*	*m*.*mm*		*P*4/*mmm a*	P_c
2	*c*				$\frac{1}{2}\frac{1}{2}0$ P_c
2	*b*	$\bar{4}2m$		*P*4/*mmm a*	$00\frac{1}{4}$ P_c
2	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c
4	*e*	222.		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*f*	2/*m*..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*g*	2.*mm*		*P*4/*mmm g*	P_c2z
4	*h*				$\frac{1}{2}\frac{1}{2}0$ P_c2z
4	*i*	*m*.2*m*	*	$P4_2/mcm$ *i*	.2. P_c2xx
4	*j*				$00\frac{1}{2}$ .2. P_c2xx
8	*k*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*l*	.2.		*P*4/*mmm l*	$00\frac{1}{4}$ P_c4x
8	*m*				$\frac{1}{2}\frac{1}{2}\frac{1}{4}$ P_c4x
8	*n*	*m*..	*	$P4_2/mcm$ *n*	.2. P_c2xx2y
8	*o*	..*m*	*	$P4_2/mcm$ *o*	.*c*. P_c2xx2z
16	*p*	1	*	$P4_2/mcm$ *p*	.*c*. $P_c2xx2y2z$

133 $P4_2/nbc$

4	*a*	222.		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*b*	222.		*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*c*	2.22		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..		*P*4/*mmm a*	C_c
8	*e*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*g*	2..		*P*4/*mmm g*	C_c2z
8	*h*	.2.		$P4_2/mcm$ *i*	$00\frac{1}{4}$ ..2 C_c2x
8	*i*				$00\frac{3}{4}$ ..2 C_c2x
8	*j*	..2		*I*4/*mcm h*	$0\frac{1}{2}0$.*b*. C_c2xx
16	*k*	1	*	$P4_2/nbc$ *k*	.22 C_c4xyz

134 $P4_2/nnm$

2	*a*	$\bar{4}2m$		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	222.		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	..2/*m*		*I*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*f*				$\frac{1}{4}\frac{1}{4}\frac{3}{4}$ *F*
4	*g*	2.*mm*		*I*4/*mmm e*	*I*2*z*
8	*h*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*i*	.2.		*I*4/*mmm i*	*I*4*x*
8	*j*				$00\frac{1}{2}$ *I*4*x*
8	*k*	..2		$P4_2/mmc$ *j*	$0\frac{1}{2}\frac{1}{4}$ .2. C_c2xx
8	*l*				$0\frac{1}{2}\frac{3}{4}$ .2. C_c2xx
8	*m*	..*m*	*	$P4_2/nnm$ *m*	..2 *I*4*xxz*
16	*n*	1	*	$P4_2/nnm$ *n*	..2 *I*4*xxz*2*y*

135 $P4_2/mbc$

4	*a*	2/*m*..		*P*4/*mmm a*	C_c
4	*b*	$\bar{4}$..		*P*4/*mmm a*	$00\frac{1}{4}$ C_c
4	*c*	2/*m*..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	2.22		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
8	*e*	2..		*P*4/*mmm g*	C_c2z
8	*f*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*g*	..2		*P*4/*mbm g*	$0\frac{1}{2}\frac{1}{4}$ (.*b*. *C*2*xx*)$_c$
8	*h*	*m*..	*	$P4_2/mbc$ *h*	.*b*2 C_c2xy
16	*i*	1	*	$P4_2/mbc$ *i*	.*b*2 C_c2xy2z

136 $P4_2/mnm$

2	*a*	*m*.*mm*		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	2/*m*..		*P*4/*mmm a*	$0\frac{1}{2}0$ C_c
4	*d*	$\bar{4}$..		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}$ C_c
4	*e*	2.*mm*		*I*4/*mmm e*	*I*2*z*
4	*f*	*m*.2*m*	*	$P4_2/mnm$ *f*	.*n*. *I*2*xx*
4	*g*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$.*n*. *I*2*xx*
8	*h*	2..		*P*4/*mmm g*	$0\frac{1}{2}0$ C_c2z
8	*i*	*m*..	*	$P4_2/mnm$ *i*	.*n*. *I*2*xx*2*y*
8	*j*	..*m*	*	$P4_2/mnm$ *j*	.*n*. *I*2*xx*2*z*
16	*k*	1	*	$P4_2/mnm$ *k*	.*n*. *I*2*xx*2*y*2*z*

137 $P4_2/nmc$

2	*a*	$\bar{4}m2$		*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}$ *I*
4	*c*	2*mm*.		*I*4/*mmm e*	*I*2*z*
4	*d*	2*mm*.		*P*4/*nmm c*	$0\frac{1}{2}0$ (..2 *CI*1*z*)$_c$
8	*e*	$\bar{1}$		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*f*	..2		*I*4/*mmm h*	*I*4*xx*
8	*g*	.*m*.	*	$P4_2/nmc$ *g*	..*c* *I*4*xz*
16	*h*	1	*	$P4_2/nmc$ *h*	..*c* *I*4*xz*2*y*

Table 3.4.3.3 (continued)

138 $P4_2/ncm$

4	*a*	2.22		*P*4/*mmm a*	$00\frac{1}{4}\ C_c$
4	*b*	$\bar{4}$..		*P*4/*mmm a*	C_c
4	*c*	..2/*m*		*I*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ F$
4	*d*				$\frac{1}{4}\frac{1}{4}\frac{3}{4}\ F$
4	*e*	2*mm*		*P*4/*nmm c*	$0\frac{1}{2}0\ (..2\ CI1z)_c$
8	*f*	2..		*P*4/*mmm g*	C_c2z
8	*g*	..2		$P4_2/mmc$ *j*	$00\frac{1}{4}\ .2.\ C_c2xx$
8	*h*				$00\frac{3}{4}\ .2.\ C_c2xx$
8	*i*	..*m*	*	$P4_2/ncm$ *i*	$\frac{1}{4}\frac{3}{4}\frac{1}{4}\ \bar{4}..\ F2xxz$
16	*j*	1	*	$P4_2/ncm$ *j*	$..m2\ C_c4xyz$

139 $I4/mmm$

2	*a*	4/*mmm*	*	*I*4/*mmm a*	*I*
2	*b*				$00\frac{1}{2}\ I$
4	*c*	*mmm*.		*P*4/*mmm a*	$0\frac{1}{2}0\ C_c$
4	*d*	$\bar{4}m2$		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}\ C_c$
4	*e*	4*mm*	*	*I*4/*mmm e*	*I*2*z*
8	*f*	..2/*m*		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*g*	2*mm*.		*P*4/*mmm g*	$0\frac{1}{2}0\ C_c2z$
8	*h*	*m*.2*m*	*	*I*4/*mmm h*	*I*4*xx*
8	*i*	*m*2*m*.	*	*I*4/*mmm i*	*I*4*x*
8	*j*				$\frac{1}{2}\frac{1}{2}0\ I4x$
16	*k*	..2		*P*4/*mmm l*	$0\frac{1}{2}\frac{1}{4}\ C_c4xx$
16	*l*	*m*..	*	*I*4/*mmm l*	*I*4*x*2*y*
16	*m*	..*m*	*	*I*4/*mmm m*	*I*4*xx*2*z*
16	*n*	.*m*.	*	*I*4/*mmm n*	*I*4*x*2*z*
32	*o*	1	*	*I*4/*mmm o*	*I*4*x*2*y*2*z*

140 $I4/mcm$

4	*a*	422		*P*4/*mmm a*	$00\frac{1}{4}\ C_c$
4	*b*	$\bar{4}2m$		*P*4/*mmm a*	$0\frac{1}{2}\frac{1}{4}\ C_c$
4	*c*	4/*m*..		*P*4/*mmm a*	C_c
4	*d*	*m*.*mm*		*P*4/*mmm a*	$0\frac{1}{2}0\ C_c$
8	*e*	..2/*m*		*P*4/*mmm a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ P_2$
8	*f*	4..		*P*4/*mmm g*	C_c2z
8	*g*	2.*mm*		*P*4/*mmm g*	$0\frac{1}{2}0\ C_c2z$
8	*h*	*m*.2*m*	*	*I*4/*mcm h*	$0\frac{1}{2}0\ .b.\ C_c2xx$
16	*i*	..2		*P*4/*mmm l*	$00\frac{1}{4}\ C_c4xx$
16	*j*	.2.		*P*4/*mmm j*	$00\frac{1}{4}\ C_c4x$
16	*k*	*m*..	*	*I*4/*mcm k*	$..m\ C_c4xy$
16	*l*	..*m*	*	*I*4/*mcm l*	$0\frac{1}{2}\frac{1}{4}\ .b.\ C_c4xxz$
32	*m*	1	*	*I*4/*mcm m*	$.c.\ C_c4xy2z$

141 $I4_1/amd$

4	*a*	$\bar{4}m2$	*	$I4_1/amd$ *a*	${}^vD$
4	*b*				$00\frac{1}{2}\ {}^vD$
8	*c*	.2/*m*.	*	$I4_1/amd$ *c*	${}^vT$
8	*d*				$00\frac{1}{2}\ {}^vT$
8	*e*	2*mm*.	*	$I4_1/amd$ *e*	${}^vD2z$
16	*f*	.2.	*	$I4_1/amd$ *f*	$..2\ {}^vT2x$
16	*g*	..2	*	$I4_1/amd$ *g*	${}^vD4xx$
16	*h*	.*m*.	*	$I4_1/amd$ *h*	$.2.\ {}^vD4xz$
32	*i*	1	*	$I4_1/amd$ *i*	$.2.\ {}^vD4xz2y$

142 $I4_1/acd$

8	*a*	$\bar{4}$..		*I*4/*mmm a*	F_c
8	*b*	2.22		*I*4/*mmm a*	$00\frac{1}{4}\ F_c$
16	*c*	$\bar{1}$		*I*4/*mmm a*	$0\frac{1}{4}\frac{1}{8}\ I_2$
16	*d*	2..		*I*4/*mmm e*	F_c2z
16	*e*	.2.	*	$I4_1/acd$ *e*	$0\frac{1}{4}\frac{3}{8}\ \bar{4}..\ I_2P_{c2}1x$
16	*f*	..2	*	$I4_1/acd$ *f*	$00\frac{1}{4}\ .2.\ F_c2xx$
32	*g*	1	*	$I4_1/acd$ *g*	$.22\ F_c4xyz$

143 $P3$

1	*a*	3..		*P*6/*mmm a*	*P*[*z*]
1	*b*				$\frac{1}{3}\frac{2}{3}0\ P[z]$
1	*c*				$\frac{2}{3}\frac{1}{3}0\ P[z]$
3	*d*	1		$P\bar{6}$ *j*	*P*3*xy*[*z*]

144 $P3_1$

3	*a*	1	*	$P3_2$ *a*	$3_1..\ P_CR^-Q1xy[z]$

145 $P3_2$

3	*a*	1	*	$P3_2$ *a*	$3_2..\ P_CR^+Q1xy[z]$

146 $R3$ (Hexagonal axes)

3	*a*	3.		$R\bar{3}m$ *a*	*R*[*z*]
9	*b*	1	*	*R*3 *b*	*R*3*xy*[*z*]

146 $R3$ (Rhombohedral axes)

1	*a*	3.		$R\bar{3}m$ *a*	*P*[*xxx*]
3	*b*	1	*	*R*3 *b*	*P*3*yz*[*xxx*]

147 $P\bar{3}$

1	*a*	$\bar{3}$..		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}\ P$
2	*c*	3..		*P*6/*mmm e*	*P*2*z*
2	*d*	3..		$P\bar{3}m1$ *d*	$.2.\ GE1z$
3	*e*	$\bar{1}$		*P*6/*mmm f*	*N*
3	*f*				$00\frac{1}{2}\ N$
6	*g*	1	*	$P\bar{3}$ *g*	*P*6*xyz*

148 $R\bar{3}$ (Hexagonal axes)

3	*a*	$\bar{3}$.		$R\bar{3}m$ *a*	*R*
3	*b*				$00\frac{1}{2}\ R$
6	*c*	3.		$R\bar{3}m$ *c*	*R*2*z*
9	*d*	$\bar{1}$		$R\bar{3}m$ *e*	$00\frac{1}{2}\ M$
9	*e*				*M*
18	*f*	1	*	$R\bar{3}$ *f*	*R*6*xyz*

148 $R\bar{3}$ (Rhombohedral axes)

1	*a*	$\bar{3}$.		$R\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*c*	3.		$R\bar{3}m$ *c*	*P*2*xxx*
3	*d*	$\bar{1}$		$R\bar{3}m$ *e*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ J$
3	*e*				*J*
6	*f*	1	*	$R\bar{3}$ *f*	*P*6*xyz*

Table 3.4.3.3 (continued)

149 *P*312

1	*a*	3.2		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
1	*c*				$\frac{1}{3}\frac{2}{3}0$ *P*
1	*d*				$\frac{1}{3}\frac{2}{3}\frac{1}{2}$ *P*
1	*e*				$\frac{2}{3}\frac{1}{3}0$ *P*
1	*f*				$\frac{2}{3}\frac{1}{3}\frac{1}{2}$ *P*
2	*g*	3..		*P*6/*mmm e*	*P*2*z*
2	*h*				$\frac{1}{3}\frac{2}{3}0$ *P*2*z*
2	*i*				$\frac{2}{3}\frac{1}{3}0$ *P*2*z*
3	*j*	..2		*P*$\bar{6}$*m*2 *j*	*P*3*x*$\bar{x}$
3	*k*				$00\frac{1}{2}$ *P*3*x*$\bar{x}$
6	*l*	1	*	*P*312 *l*	*P*3*x*$\bar{x}$2*yz*

150 *P*321

1	*a*	32.		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
2	*c*	3..		*P*6/*mmm e*	*P*2*z*
2	*d*	3..		*P*$\bar{3}$*m*1 *d*	.2. *GE*1*z*
3	*e*	.2.		*P*$\bar{6}$2*m f*	*P*3*x*
3	*f*				$00\frac{1}{2}$ *P*3*x*
6	*g*	1	*	*P*321 *g*	*P*3*x*2*yz*

151 $P3_112$

3	*a*	..2	*	$P3_112$ *a*	$00\frac{1}{3}$ 3_1.. $P_C{}^-Q1x\bar{x}$
3	*b*				$00\frac{5}{6}$ 3_1.. $P_C{}^-Q1x\bar{x}$
6	*c*	1	*	$P3_112$ *c*	$00\frac{1}{3}$ 3_1.. $P_C{}^-Q1x\bar{x}2yz$

152 $P3_121$

3	*a*	.2.	*	$P3_221$ *a*	$00\frac{1}{3}$ 3_1.. P_CR^-Q1x
3	*b*				$00\frac{5}{6}$ 3_1.. P_CR^-Q1x
6	*c*	1	*	$P3_221$ *c*	$00\frac{1}{3}$ 3_1.. $P_CR^-Q1x2yz$

153 $P3_212$

3	*a*	..2	*	$P3_112$ *a*	$00\frac{2}{3}$ 3_2.. $P_C{}^+Q1x\bar{x}$
3	*b*				$00\frac{1}{6}$ 3_2.. $P_C{}^+Q1x\bar{x}$
6	*c*	1	*	$P3_112$ *c*	$00\frac{2}{3}$ 3_2.. $P_C{}^+Q1x\bar{x}2yz$

154 $P3_221$

3	*a*	.2.	*	$P3_221$ *a*	$00\frac{2}{3}$ 3_2.. P_CR^+Q1x
3	*b*				$00\frac{1}{6}$ 3_2.. P_CR^+Q1x
6	*c*	1	*	$P3_221$ *c*	$00\frac{2}{3}$ 3_2.. $P_CR^+Q1x2yz$

155 *R*32 (Hexagonal axes)

3	*a*	32		*R*$\bar{3}$*m a*	*R*
3	*b*				$00\frac{1}{2}$ *R*
6	*c*	3.		*R*$\bar{3}$*m c*	*R*2*z*
9	*d*	.2	*	*R*32 *d*	*R*3*x*
9	*e*				$00\frac{1}{2}$ *R*3*x*
18	*f*	1	*	*R*32 *f*	*R*3*x*2*yz*

155 *R*32 (Rhombohedral axes)

1	*a*	32		*R*$\bar{3}$*m a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
2	*c*	3.		*R*$\bar{3}$*m c*	*P*2*xxx*
3	*d*	.2	*	*R*32 *d*	*P*3*x*$\bar{x}$
3	*e*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*3*x*$\bar{x}$
6	*f*	1	*	*R*32 *f*	*P*3*x*$\bar{x}$2*yz*

156 *P*3*m*1

1	*a*	3*m*.		*P*6/*mmm a*	*P*[*z*]
1	*b*				$\frac{1}{3}\frac{2}{3}0$ *P*[*z*]
1	*c*				$\frac{2}{3}\frac{1}{3}0$ *P*[*z*]
3	*d*	.*m*.		*P*$\bar{6}$*m*2 *j*	*P*3*x*$\bar{x}$[*z*]
6	*e*	1		*P*$\bar{6}$*m*2 *l*	*P*3*x*$\bar{x}$2*y*[*z*]

157 *P*31*m*

1	*a*	3.*m*		*P*6/*mmm a*	*P*[*z*]
2	*b*	3..		*P*6/*mmm c*	*G*[*z*]
3	*c*	..*m*		*P*$\bar{6}$2*m f*	*P*3*x*[*z*]
6	*d*	1		*P*$\bar{6}$2*m j*	*P*3*x*2*y*[*z*]

158 *P*3*c*1

2	*a*	3..		*P*6/*mmm a*	P_c[*z*]
2	*b*				$\frac{1}{3}\frac{2}{3}0$ P_c[*z*]
2	*c*				$\frac{2}{3}\frac{1}{3}0$ P_c[*z*]
6	*d*	1		*P*$\bar{6}$*c*2 *k*	..2 P_c3*xy*[*z*]

159 *P*31*c*

2	*a*	3..		*P*6/*mmm a*	P_c[*z*]
2	*b*	3..		*P*6$_3$/*mmc c*	*E*[*z*]
6	*c*	1		*P*$\bar{6}$2*c h*	.2. P_c3*xy*[*z*]

160 *R*3*m* (Hexagonal axes)

3	*a*	3*m*		*R*$\bar{3}$*m a*	*R*[*z*]
9	*b*	.*m*	*	*R*3*m b*	*R*3*x*$\bar{x}$[*z*]
18	*c*	1	*	*R*3*m c*	*R*3*x*$\bar{x}$2*y*[*z*]

160 *R*3*m* (Rhombohedral axes)

1	*a*	3*m*		*R*$\bar{3}$*m a*	*P*[*xxx*]
3	*b*	.*m*	*	*R*3*m b*	*P*3*z*[*xxx*]
6	*c*	1	*	*R*3*m c*	*P*3*z*2*y*[*xxx*]

161 *R*3*c* (Hexagonal axes)

6	*a*	3.		*R*$\bar{3}$*m a*	$'R_c$[*z*]
18	*b*	1	*	*R*3*c b*	.*c* $'R_c$3*xy*[*z*]

161 *R*3*c* (Rhombohedral axes)

2	*a*	3.		*R*$\bar{3}$*m a*	*I*[*xxx*]
6	*b*	1	*	*R*3*c b*	.*n I*3*yz*[*xxx*]

162 *P*$\bar{3}$1*m*

1	*a*	$\bar{3}$.*m*		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
2	*c*	3.2		*P*6/*mmm c*	*G*
2	*d*				$00\frac{1}{2}$ *G*
2	*e*	3.*m*		*P*6/*mmm e*	*P*2*z*
3	*f*	..2/*m*		*P*6/*mmm f*	*N*

Table 3.4.3.3 (continued)

3	*g*				$00\frac{1}{2}\ N$
4	*h*	3..		*P*6/*mmm h*	*G*2*z*
6	*i*	..2		*P*6/*mmm l*	$P6x\bar{x}$
6	*j*				$00\frac{1}{2}\ P6x\bar{x}$
6	*k*	..*m*	*	$P\bar{3}1m\ k$	*P*6*xz*
12	*l*	1	*	$P\bar{3}1m\ l$	*P*6*xz*2*y*

163 $P\bar{3}1c$

2	*a*	3.2		*P*6/*mmm a*	$00\frac{1}{4}\ P_c$
2	*b*	$\bar{3}$..		*P*6/*mmm a*	P_c
2	*c*	3.2		$P6_3/mmc\ c$	*E*
2	*d*				$00\frac{1}{2}\ E$
4	*e*	3..		*P*6/*mmm e*	P_c2z
4	*f*	3..		$P6_3/mmc\ f$	*E*2*z*
6	*g*	$\bar{1}$		*P*6/*mmm f*	N_c
6	*h*	..2		$P6_3/mmc\ h$	$00\frac{1}{4}\ .2.\ P_c3x\bar{x}$
12	*i*	1	*	$P\bar{3}1c\ i$	$..c\ P_c6xyz$

164 $P\bar{3}m1$

1	*a*	$\bar{3}m.$		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}\ P$
2	*c*	3*m*.		*P*6/*mmm e*	*P*2*z*
2	*d*	3*m*.	*	$P\bar{3}m1\ d$	$.2.\ GE1z$
3	*e*	.2/*m*.		*P*6/*mmm f*	*N*
3	*f*				$00\frac{1}{2}\ N$
6	*g*	.2.		*P*6/*mmm j*	*P*6*x*
6	*h*				$00\frac{1}{2}\ P6x$
6	*i*	.*m*.	*	$P\bar{3}m1\ i$	$P6x\bar{x}z$
12	*j*	1	*	$P\bar{3}m1\ j$	$P6x\bar{x}z2y$

165 $P\bar{3}c1$

2	*a*	32.		*P*6/*mmm a*	$00\frac{1}{4}\ P_c$
2	*b*	$\bar{3}$..		*P*6/*mmm a*	P_c
4	*c*	3..		*P*6/*mmm e*	P_c2z
4	*d*	3..		$P\bar{3}m1\ d$	$(.2.\ GE1z)_c$
6	*e*	$\bar{1}$		*P*6/*mmm f*	N_c
6	*f*	.2.		$P6_3/mcm\ g$	$00\frac{1}{4}\ ..2\ P_c3x$
12	*g*	1	*	$P\bar{3}c1\ g$	$.c.\ P_c6xyz$

166 $R\bar{3}m$ (Hexagonal axes)

3	*a*	$\bar{3}m$	*	$R\bar{3}m\ a$	*R*
3	*b*				$00\frac{1}{2}\ R$
6	*c*	3*m*	*	$R\bar{3}m\ c$	*R*2*z*
9	*e*	.2/*m*	*	$R\bar{3}m\ e$	*M*
9	*d*				$00\frac{1}{2}\ M$
18	*f*	.2	*	$R\bar{3}m\ f$	*R*6*x*
18	*g*				$00\frac{1}{2}\ R6x$
18	*h*	.*m*	*	$R\bar{3}m\ h$	$R6x\bar{x}z$
36	*i*	1	*	$R\bar{3}m\ i$	$R6x\bar{x}z2y$

166 $R\bar{3}m$ (Rhombohedral axes)

1	*a*	$\bar{3}m$	*	$R\bar{3}m\ a$	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P$
2	*c*	3*m*	*	$R\bar{3}m\ c$	*P*2*xxx*
3	*e*	.2/*m*	*	$R\bar{3}m\ e$	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ J$
6	*f*	.2	*	$R\bar{3}m\ f$	$P6x\bar{x}$
6	*g*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}\ P6x\bar{x}$
6	*h*	.*m*	*	$R\bar{3}m\ h$	*P*6*xxz*
12	*i*	1	*	$R\bar{3}m\ i$	*P*6*xxz*2*y*

167 $R\bar{3}c$ (Hexagonal axes)

6	*a*	32		$R\bar{3}m\ a$	$00\frac{1}{4}\ {}'R_c$
6	*b*	$\bar{3}$.		$R\bar{3}m\ a$	${}'R_c$
12	*c*	3.		$R\bar{3}m\ c$	${}'R_c2z$
18	*d*	$\bar{1}$		$R\bar{3}m\ e$	${}'M_c$
18	*e*	.2	*	$R\bar{3}c\ e$	$00\frac{1}{4}\ .c\ {}'R_c3x$
36	*f*	1	*	$R\bar{3}c\ f$	$.c\ {}'R_c6xyz$

167 $R\bar{3}c$ (Rhombohedral axes)

2	*a*	32		$R\bar{3}m\ a$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ I$
2	*b*	$\bar{3}$.		$R\bar{3}m\ a$	*I*
4	*c*	3.		$R\bar{3}m\ c$	*I*2*xxx*
6	*d*	$\bar{1}$		$R\bar{3}m\ e$	J^*
6	*e*	.2	*	$R\bar{3}c\ e$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}\ .n\ I3x\bar{x}$
12	*f*	1	*	$R\bar{3}c\ f$	*.n I*6*xyz*

168 *P*6

1	*a*	6..		*P*6/*mmm a*	*P*[*z*]
2	*b*	3..		*P*6/*mmm c*	*G*[*z*]
3	*c*	2..		*P*6/*mmm f*	*N*[*z*]
6	*d*	1		*P*6/*m j*	*P*6*xy*[*z*]

169 $P6_1$

6	*a*	1	*	$P6_1\ a$	$3_12_1..\ P_{Cc}E_C{}^+Q_c1xy[z]$

170 $P6_5$

6	*a*	1	*	$P6_1a$	$3_22_1..\ P_{Cc}E_C{}^-Q_c1xy[z]$

171 $P6_2$

3	*a*	2..		*P*6/*mmm a*	$P_C[z]$
3	*b*	2..		$P6_222\ c$	${}^+Q[z]$
6	*c*	1	*	$P6_2\ c$	$3_2..\ P_C2xy[z]$

172 $P6_4$

3	*a*	2..		*P*6/*mmm a*	$P_C[z]$
3	*b*	2..		$P6_222\ c$	${}^-Q[z]$
6	*c*	1	*	$P6_2\ c$	$3_1..\ P_C2xy[z]$

173 $P6_3$

2	*a*	3..		*P*6/*mmm a*	$P_c[z]$
2	*b*	3..		$P6_3/mmc\ c$	*E*[*z*]
6	*c*	1		$P6_3/m\ h$	$2_1..\ P_c3xy[z]$

174 $P\bar{6}$

1	*a*	$\bar{6}$..		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}\ P$
1	*c*				$\frac{1}{3}\frac{2}{3}0\ P$

Table 3.4.3.3 (continued)

1	*d*				$\frac{1}{3}\frac{2}{3}\frac{1}{2}$ *P*
1	*e*				$\frac{2}{3}\frac{1}{3}0$ *P*
1	*f*				$\frac{2}{3}\frac{1}{3}\frac{1}{2}$ *P*
2	*g*	3..		*P*6/*mmm e*	*P*2*z*
2	*h*				$\frac{1}{3}\frac{2}{3}0$ *P*2*z*
2	*i*				$\frac{2}{3}\frac{1}{3}0$ *P*2*z*
3	*j*	*m*..	*	$P\bar{6}$ *j*	*P*3*xy*
3	*k*				$00\frac{1}{2}$ *P*3*xy*
6	*l*	1	*	$P\bar{6}$ *l*	*P*3*xy*2*z*

175 *P*6/*m*

1	*a*	6/*m*..		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
2	*c*	$\bar{6}$..		*P*6/*mmm c*	*G*
2	*d*				$00\frac{1}{2}$ *G*
2	*e*	6..		*P*6/*mmm e*	*P*2*z*
3	*f*	2/*m*..		*P*6/*mmm f*	*N*
3	*g*				$00\frac{1}{2}$ *N*
4	*h*	3..		*P*6/*mmm h*	*G*2*z*
6	*i*	2..		*P*6/*mmm i*	*N*2*z*
6	*j*	*m*..	*	*P*6/*m j*	*P*6*xy*
6	*k*				$00\frac{1}{2}$ *P*6*xy*
12	*l*	1	*	*P*6/*m l*	*P*6*xy*2*z*

176 $P6_3/m$

2	*a*	$\bar{6}$..		*P*6/*mmm a*	$00\frac{1}{4}$ P_c
2	*b*	$\bar{3}$..		*P*6/*mmm a*	P_c
2	*c*	$\bar{6}$..		$P6_3/mmc$ *c*	*E*
2	*d*				$00\frac{1}{2}$ *E*
4	*e*	3..		*P*6/*mmm e*	P_c2*z*
4	*f*	3..		$P6_3/mmc$ *f*	*E*2*z*
6	*g*	$\bar{1}$		*P*6/*mmm f*	N_c
6	*h*	*m*..	*	$P6_3/m$ *h*	$00\frac{1}{4}$ 2_1.. P_c3*xy*
12	*i*	1	*	$P6_3/m$ *i*	*m*.. P_c6*xyz*

177 *P*622

1	*a*	622		*P*6/*mmm a*	*P*
1	*b*				$00\frac{1}{2}$ *P*
2	*c*	3.2		*P*6/*mmm c*	*G*
2	*d*				$00\frac{1}{2}$ *G*
2	*e*	6..		*P*6/*mmm e*	*P*2*z*
3	*f*	222		*P*6/*mmm f*	*N*
3	*g*				$00\frac{1}{2}$ *N*
4	*h*	3..		*P*6/*mmm h*	*G*2*z*
6	*i*	2..		*P*6/*mmm i*	*N*2*z*
6	*j*	.2.		*P*6/*mmm j*	*P*6*x*
6	*k*				$00\frac{1}{2}$ *P*6*x*
6	*l*	..2		*P*6/*mmm l*	*P*6*x*$\bar{x}$
6	*m*				$00\frac{1}{2}$ *P*6*x*$\bar{x}$
12	*n*	1	*	*P*622 *n*	*P*6*x*2*yz*

178 $P6_122$

6	*a*	.2.	*	$P6_122$ *a*	3_1.2 $P_{Cc}{}^{+}Q_c1x$
6	*b*	..2	*	$P6_122$ *b*	$00\frac{11}{12}$ $3_1$2. $P_{Cc}E_C{}^{+}Q_c1x\bar{x}$
12	*c*	1	*	$P6_122$ *c*	3_1.2 $P_{Cc}{}^{+}Q_c1x2yz$

179 $P6_522$

6	*a*	.2.	*	$P6_122$ *a*	3_2.2 $P_{Cc}{}^{-}Q_c1x$
6	*b*	..2	*	$P6_122$ *b*	$00\frac{1}{12}$ $3_2$2. $P_{Cc}E_C{}^{-}Q_c1x\bar{x}$
12	*c*	1	*	$P6_122$ *c*	3_2.2 $P_{Cc}{}^{-}Q_c1x2yz$

180 $P6_222$

3	*a*	222		*P*6/*mmm a*	P_C
3	*b*				$00\frac{1}{2}$ P_C
3	*c*	222	*	$P6_222$ *c*	^{+}Q
3	*d*				$00\frac{1}{2}$ ^{+}Q
6	*e*	2..		*P*6/*mmm e*	P_C2*z*
6	*f*	2..	*	$P6_222$ *f*	^{+}Q2*z*
6	*g*	.2.	*	$P6_222$ *g*	3_2.. P_C2*x*
6	*h*				$00\frac{1}{2}$ 3_2.. P_C2*x*
6	*i*	..2	*	$P6_222$ *i*	$00\frac{1}{3}$ 3_2.. P_C2*x*$\bar{x}$
6	*j*				$00\frac{5}{6}$ 3_2.. P_C2*x*$\bar{x}$
12	*k*	1	*	$P6_222$ *k*	3_2.. P_C2*x*2*yz*

181 $P6_422$

3	*a*	222		*P*6/*mmm a*	P_C
3	*b*				$00\frac{1}{2}$ P_C
3	*c*	222	*	$P6_222$ *c*	^{-}Q
3	*d*				$00\frac{1}{2}$ ^{-}Q
6	*e*	2..		*P*6/*mmm e*	P_C2*z*
6	*f*	2..	*	$P6_222$ *f*	^{-}Q2*z*
6	*g*	.2.	*	$P6_222$ *g*	3_1.. P_C2*x*
6	*h*				$00\frac{1}{2}$ 3_1.. P_C2*x*
6	*i*	..2	*	$P6_222$ *i*	$00\frac{2}{3}$ 3_1.. P_C2*x*$\bar{x}$
6	*j*				$00\frac{1}{6}$ 3_1.. P_C2*x*$\bar{x}$
12	*k*	1	*	$P6_222$ *k*	3_1.. P_C2*x*2*yz*

182 $P6_322$

2	*a*	32.		*P*6/*mmm a*	P_c
2	*b*	3.2		*P*6/*mmm a*	$00\frac{1}{4}$ P_c
2	*c*	3.2		$P6_3/mmc$ *c*	*E*
2	*d*				$00\frac{1}{2}$ *E*
4	*e*	3..		*P*6/*mmm e*	P_c2*z*
4	*f*	3..		$P6_3/mmc$ *f*	*E*2*z*
6	*g*	.2.		$P6_3/mcm$ *g*	..2 P_c3*x*
6	*h*	..2		$P6_3/mmc$ *h*	$00\frac{1}{4}$ .2. P_c3*x*$\bar{x}$
12	*i*	1	*	$P6_322$ *i*	..2 P_c3*x*2*yz*

183 *P*6*mm*

1	*a*	6*mm*		*P*6/*mmm a*	*P*[*z*]
2	*b*	3*m*.		*P*6/*mmm c*	*G*[*z*]
3	*c*	2*mm*		*P*6/*mmm f*	*N*[*z*]
6	*d*	..*m*		*P*6/*mmm j*	*P*6*x*[*z*]
6	*e*	.*m*.		*P*6/*mmm l*	*P*6*x*$\bar{x}$[*z*]
12	*f*	1		*P*6/*mmm p*	*P*6*x*2*y*[*z*]

Table 3.4.3.3 (continued)

184 *P6cc*

2	*a*	6..		*P6/mmm a*	$P_c[z]$
4	*b*	3..		*P6/mmm c*	$G_c[z]$
6	*c*	2..		*P6/mmm f*	$N_c[z]$
12	*d*	1		*P6/mcc l*	$.c.\ P_c6xy[z]$

185 *P6$_3$cm*

2	*a*	3*m*		*P6/mmm a*	$P_c[z]$
4	*b*	3..		*P6/mmm c*	$G_c[z]$
6	*c*	*..m*		*P6$_3$/mcm g*	$..2\ P_c3x[z]$
12	*d*	1		*P6$_3$/mcm j*	$..2\ P_c3x2y[z]$

186 *P6$_3$mc*

2	*a*	3*m*.		*P6/mmm a*	$P_c[z]$
2	*b*	3*m*.		*P6$_3$/mmc c*	$E[z]$
6	*c*	*.m*.		*P6$_3$/mmc h*	$.2.\ P_c3x\bar{x}[z]$
12	*d*	1		*P6$_3$/mmc j*	$.2.\ P_c3x\bar{x}2y[z]$

187 *P$\bar{6}$m2*

1	*a*	$\bar{6}$*m*2		*P6/mmm a*	*P*
1	*b*				$00\frac{1}{2}\ P$
1	*c*				$\frac{1}{3}\frac{2}{3}0\ P$
1	*d*				$\frac{1}{3}\frac{2}{3}\frac{1}{2}\ P$
1	*e*				$\frac{2}{3}\frac{1}{3}0\ P$
1	*f*				$\frac{2}{3}\frac{1}{3}\frac{1}{2}\ P$
2	*g*	3*m*.		*P6/mmm e*	*P2z*
2	*h*				$\frac{1}{3}\frac{2}{3}0\ P2z$
2	*i*				$\frac{2}{3}\frac{1}{3}0\ P2z$
3	*j*	*mm*2	*	*P$\bar{6}$m2 j*	$P3x\bar{x}$
3	*k*				$00\frac{1}{2}\ P3x\bar{x}$
6	*l*	*m*..	*	*P$\bar{6}$m2 l*	$P3x\bar{x}2y$
6	*m*				$00\frac{1}{2}\ P3x\bar{x}2y$
6	*n*	*.m*.	*	*P$\bar{6}$m2 n*	$P3x\bar{x}2z$
12	*o*	1	*	*P$\bar{6}$m2 o*	$P3x\bar{x}2y2z$

188 *P$\bar{6}$c2*

2	*a*	3.2		*P6/mmm a*	P_c
2	*c*				$\frac{1}{3}\frac{2}{3}0\ P_c$
2	*e*				$\frac{2}{3}\frac{1}{3}0\ P_c$
2	*b*	$\bar{6}$..		*P6/mmm a*	$00\frac{1}{4}\ P_c$
2	*d*				$\frac{1}{3}\frac{2}{3}\frac{1}{4}\ P_c$
2	*f*				$\frac{2}{3}\frac{1}{3}\frac{1}{4}\ P_c$
4	*g*	3..		*P6/mmm e*	P_c2z
4	*h*				$\frac{1}{3}\frac{2}{3}0\ P_c2z$
4	*i*				$\frac{2}{3}\frac{1}{3}0\ P_c2z$
6	*j*	*..2*		*P$\bar{6}$m2 j*	$P_c3x\bar{x}$
6	*k*	*m*..	*	*P$\bar{6}$c2 k*	$00\frac{1}{4}\ ..2\ P_c3xy$
12	*l*	1	*	*P$\bar{6}$c2 l*	$m..\ P_c3x\bar{x}2yz$

189 *P$\bar{6}$2m*

1	*a*	$\bar{6}$2*m*		*P6/mmm a*	*P*
1	*b*				$00\frac{1}{2}\ P$
2	*c*	$\bar{6}$..		*P6/mmm c*	*G*
2	*d*				$00\frac{1}{2}\ G$
2	*e*	3.*m*		*P6/mmm e*	*P2z*
3	*f*	*m*2*m*	*	*P$\bar{6}$2m f*	*P3x*
3	*g*				$00\frac{1}{2}\ P3x$
4	*h*	3..		*P6/mmm h*	*G2z*
6	*i*	*..m*	*	*P$\bar{6}$2m i*	*P3x2z*
6	*j*	*m*..	*	*P$\bar{6}$2m j*	*P3x2y*
6	*k*				$00\frac{1}{2}\ P3x2y$
12	*l*	1	*	*P$\bar{6}$2m l*	*P3x2y2z*

190 *P$\bar{6}$2c*

2	*a*	32.		*P6/mmm a*	P_c
2	*b*	$\bar{6}$..		*P6/mmm a*	$00\frac{1}{4}\ P_c$
2	*c*	$\bar{6}$..		*P6$_3$/mmc c*	*E*
2	*d*				$00\frac{1}{2}\ E$
4	*e*	3..		*P6/mmm e*	P_c2z
4	*f*	3..		*P6$_3$/mmc f*	*E2z*
6	*g*	.2.		*P$\bar{6}$2m f*	P_c3x
6	*h*	*m*..	*	*P$\bar{6}$2c h*	$00\frac{1}{4}\ .2.\ P_c3xy$
12	*i*	1	*	*P$\bar{6}$2c i*	$m..\ P_c3x2yz$

191 *P6/mmm*

1	*a*	6/*mmm*	*	*P6/mmm a*	*P*
1	*b*				$00\frac{1}{2}\ P$
2	*c*	$\bar{6}$*m*2	*	*P6/mmm c*	*G*
2	*d*				$00\frac{1}{2}\ G$
2	*e*	6*mm*	*	*P6/mmm e*	*P2z*
3	*f*	*mmm*	*	*P6/mmm f*	*N*
3	*g*				$00\frac{1}{2}\ N$
4	*h*	3*m*.	*	*P6/mmm h*	*G2z*
6	*i*	2*mm*	*	*P6/mmm i*	*N2z*
6	*j*	*m*2*m*	*	*P6/mmm j*	*P6x*
6	*k*				$00\frac{1}{2}\ P6x$
6	*l*	*mm*2	*	*P6/mmm l*	$P6x\bar{x}$
6	*m*				$00\frac{1}{2}\ P6x\bar{x}$
12	*n*	*..m*	*	*P6/mmm n*	*P6x2z*
12	*o*	*.m*.	*	*P6/mmm o*	$P6x\bar{x}2z$
12	*p*	*m*..	*	*P6/mmm p*	*P6x2y*
12	*q*				$00\frac{1}{2}\ P6x2y$
24	*r*	1	*	*P6/mmm r*	*P6x2y2z*

192 *P6/mcc*

2	*a*	622		*P6/mmm a*	$00\frac{1}{4}\ P_c$
2	*b*	6/*m*..		*P6/mmm a*	P_c
4	*c*	3.2		*P6/mmm c*	$00\frac{1}{4}\ G_c$
4	*d*	$\bar{6}$..		*P6/mmm c*	G_c
4	*e*	6..		*P6/mmm e*	P_c2z
6	*f*	222		*P6/mmm f*	$00\frac{1}{4}\ N_c$
6	*g*	2/*m*..		*P6/mmm f*	N_c
8	*h*	3..		*P6/mmm h*	G_c2z
12	*i*	2..		*P6/mmm i*	N_c2z
12	*j*	.2.		*P6/mmm j*	$00\frac{1}{4}\ P_c6x$
12	*k*	*..2*		*P6/mmm l*	$00\frac{1}{4}\ P_c6x\bar{x}$
12	*l*	*m*..	*	*P6/mcc l*	$.c.\ P_c6xy$
24	*m*	1	*	*P6/mcc m*	$.c.\ P_c6xy2z$

Table 3.4.3.3 (continued)

193 $P6_3/mcm$

2	*a*	$\bar{6}2m$		$P6/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*b*	$\bar{3}.m$		$P6/mmm$ *a*	P_c
4	*c*	$\bar{6}..$		$P6/mmm$ *c*	$00\frac{1}{4}$ G_c
4	*d*	3.2		$P6/mmm$ *c*	G_c
4	*e*	3.*m*		$P6/mmm$ *e*	P_c2z
6	*f*	..2/*m*		$P6/mmm$ *f*	N_c
6	*g*	*m*2*m*	*	$P6_3/mcm$ *g*	$00\frac{1}{4}$ ..2 P_c3x
8	*h*	3..		$P6/mmm$ *h*	G_c2z
12	*i*	..2		$P6/mmm$ *l*	$P_c6x\bar{x}$
12	*j*	*m*..	*	$P6_3/mcm$ *j*	$00\frac{1}{4}$ ..2 P_c3x2y
12	*k*	..*m*	*	$P6_3/mcm$ *k*	*m*.. P_c6xz
24	*l*	1	*	$P6_3/mcm$ *l*	*m*.. P_c6xz2y

194 $P6_3/mmc$

2	*a*	$\bar{3}m.$		$P6/mmm$ *a*	P_c
2	*b*	$\bar{6}m2$		$P6/mmm$ *a*	$00\frac{1}{4}$ P_c
2	*c*	$\bar{6}m2$	*	$P6_3/mmc$ *c*	*E*
2	*d*				$00\frac{1}{2}$ *E*
4	*e*	3*m*.		$P6/mmm$ *e*	P_c2z
4	*f*	3*m*.	*	$P6_3/mmc$ *f*	*E*2*z*
6	*g*	.2/*m*.		$P6/mmm$ *f*	N_c
6	*h*	*mm*2	*	$P6_3/mmc$ *h*	$00\frac{1}{4}$ .2. $P_c3x\bar{x}$
12	*i*	.2.		$P6/mmm$ *j*	P_c6x
12	*j*	*m*..	*	$P6_3/mmc$ *j*	$00\frac{1}{4}$ .2. $P_c3x\bar{x}2y$
12	*k*	.*m*.	*	$P6_3/mmc$ *k*	*m*.. $P_c6x\bar{x}z$
24	*l*	1	*	$P6_3/mmc$ *l*	*m*.. $P_c6x\bar{x}z2y$

195 $P23$

1	*a*	23.		$Pm\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	222..		$Pm\bar{3}m$ *c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
4	*e*	.3.		$P\bar{4}3m$ *e*	*P*4*xxx*
6	*f*	2..		$Pm\bar{3}m$ *e*	*P*6*z*
6	*i*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
6	*g*	2..		$Pm\bar{3}$ *f*	.3. *J*2*x*
6	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *J*2*x*
12	*j*	1	*	*P*23 *j*	*P*6*z*2*xy*

196 $F23$

4	*a*	23.		$Fm\bar{3}m$ *a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
4	*c*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
16	*e*	.3.		$F\bar{4}3m$ *e*	*F*4*xxx*
24	*f*	2..		$Fm\bar{3}m$ *e*	*F*6*z*
24	*g*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*6*z*
48	*h*	1	*	*F*23 *h*	*F*6*z*2*xy*

197 $I23$

2	*a*	23.		$Im\bar{3}m$ *a*	*I*
6	*b*	222..		$Im\bar{3}m$ *b*	J^*
8	*c*	.3.		$I\bar{4}3m$ *c*	*I*4*xxx*
12	*d*	2..		$Im\bar{3}m$ *e*	*I*6*z*
12	*e*	2..		$Im\bar{3}$ *e*	.3. J^*2x
24	*f*	1	*	*I*23 *f*	*I*6*z*2*xy*

198 $P2_13$

4	*a*	.3.	*	$P2_13$ *a*	2_12_1.. *FY*1*xxx*
12	*b*	1	*	$P2_13$ *b*	2_12_1.. *FY*1*xxx*3*yz*

199 $I2_13$

8	*a*	.3.	*	$I2_13$ *a*	2_12_1.. P_2Y^*1xxx
12	*b*	2..	*	$I2_13$ *b*	2_13. *SV*1*z*
24	*c*	1	*	$I2_13$ *c*	2_12_1.. $P_2Y^*1xxx3yz$

200 $Pm\bar{3}$

1	*a*	$m\bar{3}.$		$Pm\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	*mmm*..		$Pm\bar{3}m$ *c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
6	*e*	*mm*2..		$Pm\bar{3}m$ *e*	*P*6*z*
6	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
6	*f*	*mm*2..	*	$Pm\bar{3}$ *f*	.3. *J*2*x*
6	*g*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *J*2*x*
8	*i*	.3.		$Pm\bar{3}m$ *g*	*P*8*xxx*
12	*j*	*m*..	*	$Pm\bar{3}$ *j*	*P*6*z*2*x*
12	*k*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*2*x*
24	*l*	1	*	$Pm\bar{3}$ *l*	*P*6*z*2*x*2*y*

201 $Pn\bar{3}$

2	*a*	23.		$Im\bar{3}m$ *a*	*I*
4	*b*	.$\bar{3}$.		$Fm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*c*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
6	*d*	222..		$Im\bar{3}m$ *b*	J^*
8	*e*	.3.		$Pn\bar{3}m$ *e*	..2 *I*4*xxx*
12	*f*	2..		$Im\bar{3}m$ *e*	*I*6*z*
12	*g*	2..		$Im\bar{3}$ *e*	.3. J^*2x
24	*h*	1	*	$Pn\bar{3}$ *h*	*n*.. *I*6*z*2*xy*

202 $Fm\bar{3}$

4	*a*	$m\bar{3}.$		$Fm\bar{3}m$ *a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	23.		$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*d*	2/*m*..		$Pm\bar{3}m$ *c*	J_2
24	*e*	*mm*2..		$Fm\bar{3}m$ *e*	*F*6*z*
32	*f*	.3.		$Fm\bar{3}m$ *f*	*F*8*xxx*
48	*g*	2..		$Pm\bar{3}m$ *e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2$6*z*
48	*h*	*m*..	*	$Fm\bar{3}$ *h*	*F*6*z*2*x*
96	*i*	1	*	$Fm\bar{3}$ *i*	*F*6*z*2*x*2*y*

203 $Fd\bar{3}$

8	*a*	23.		$Fd\bar{3}m$ *a*	*D*
8	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *D*
16	*c*	.$\bar{3}$.		$Fd\bar{3}m$ *c*	*T*
16	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *T*
32	*e*	.3.		$Fd\bar{3}m$ *e*	..2 *D*4*xxx*

Table 3.4.3.3 (continued)

48	*f*	2..		*Fd*$\bar{3}$*m f*	*D6z*
96	*g*	1	*	*Fd*$\bar{3}$ *g*	*d.. D6z2xy*

204 *Im*$\bar{3}$

2	*a*	*m*$\bar{3}$.		*Im*$\bar{3}$*m a*	*I*
6	*b*	*mmm..		*Im*$\bar{3}$*m b*	*J**
8	*c*	.$\bar{3}$.		*Pm*$\bar{3}$*m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	*mm2..		*Im*$\bar{3}$*m e*	*I6z*
12	*e*	*mm2..	*	*Im*$\bar{3}$ *e*	*.3. J*2x*
16	*f*	.3.		*Im*$\bar{3}$*m f*	*I8xxx*
24	*g*	*m..	*	*Im*$\bar{3}$ *g*	*I6z2x*
48	*h*	1	*	*Im*$\bar{3}$ *h*	*I6z2x2y*

205 *Pa*$\bar{3}$

4	*a*	.$\bar{3}$.		*Fm*$\bar{3}$*m a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	.3.	*	*Pa*$\bar{3}$ *c*	*bc.. F2xxx*
24	*d*	1	*	*Pa*$\bar{3}$ *d*	*bc.. F6xyz*

206 *Ia*$\bar{3}$

8	*a*	.$\bar{3}$.		*Pm*$\bar{3}$*m a*	P_2
8	*b*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
16	*c*	.3.	*	*Ia*$\bar{3}$ *c*	22.. $P_2$2xxx
24	*d*	2..	*	*Ia*$\bar{3}$ *d*	.$\bar{3}$. J_2*S*V*1x
48	*e*	1	*	*Ia*$\bar{3}$ *e*	22.. $P_2$6xyz

207 *P*432

1	*a*	432		*Pm*$\bar{3}$*m a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	42.2		*Pm*$\bar{3}$*m c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
6	*e*	4..		*Pm*$\bar{3}$*m e*	*P6z*
6	*f*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P6z*
8	*g*	.3.		*Pm*$\bar{3}$*m g*	*P8xxx*
12	*h*	2..		*Pm*$\bar{3}$*m h*	*.3. J4x*
12	*i*	..2		*Pm*$\bar{3}$*m i*	*P12xx*
12	*j*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P12xx*
24	*k*	1	*	*P432 k*	*P6z4xy*

208 *P*$4_2$32

2	*a*	23.		*Im*$\bar{3}$*m a*	*I*
4	*b*	.32		*Fm*$\bar{3}$*m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*c*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
6	*d*	222..		*Im*$\bar{3}$*m b*	*J**
6	*e*	2.22		*Pm*$\bar{3}$*n c*	*W*
6	*f*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *W*
8	*g*	.3.		*Pn*$\bar{3}$*m e*	*..2 I4xxx*
12	*h*	2..		*Im*$\bar{3}$*m e*	*I6z*
12	*i*	2..		*Pm*$\bar{3}$*n g*	*.3. W2z*
12	*j*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *.3. W2z*
12	*k*	..2	*	*P*$4_2$32 *k*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 4_2.. *F3x*$\bar{x}$
12	*l*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ 4_2.. *F3x*$\bar{x}$
24	*m*	1	*	*P*$4_2$32 *m*	*..2 I6z2xy*

209 *F*432

4	*a*	432		*Fm*$\bar{3}$*m a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	23.		*Pm*$\bar{3}$*m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*d*	2.22		*Pm*$\bar{3}$*m c*	J_2
24	*e*	4..		*Fm*$\bar{3}$*m e*	*F6z*
32	*f*	.3.		*Fm*$\bar{3}$*m f*	*F8xxx*
48	*g*	..2		*Fm*$\bar{3}$*m h*	*F12xx*
48	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F12xx*
48	*i*	2..		*Pm*$\bar{3}$*m e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2$6z
96	*j*	1	*	*F432 j*	*F6z4xy*

210 *F*$4_1$32

8	*a*	23.		*Fd*$\bar{3}$*m a*	*D*
8	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *D*
16	*c*	.32		*Fd*$\bar{3}$*m c*	*T*
16	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *T*
32	*e*	.3.		*Fd*$\bar{3}$*m e*	*..2 D4xxx*
48	*f*	2..		*Fd*$\bar{3}$*m f*	*D6z*
48	*g*	..2	*	*F*$4_1$32 *g*	22.. *T3x*$\bar{x}$
96	*h*	1	*	*F*$4_1$32 *h*	*..2 D6z2xy*

211 *I*432

2	*a*	432		*Im*$\bar{3}$*m a*	*I*
6	*b*	42.2		*Im*$\bar{3}$*m b*	*J**
8	*c*	.32		*Pm*$\bar{3}$*m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	2.22		*Im*$\bar{3}$*m d*	*W**
12	*e*	4..		*Im*$\bar{3}$*m e*	*I6z*
16	*f*	.3.		*Im*$\bar{3}$*m f*	*I8xxx*
24	*g*	2..		*Im*$\bar{3}$*m g*	*.3. J*4x*
24	*h*	..2		*Im*$\bar{3}$*m h*	*I12xx*
24	*i*	..2	*	*I432 i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ 4.. $P_2$3x$\bar{x}$
48	*j*	1	*	*I432 j*	*I6z4xy*

212 *P*$4_3$32

4	*a*	.32	*	*P*$4_3$32 *a*	^{+}Y
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ^{+}Y
8	*c*	.3.	*	*P*$4_3$32 *c*	4_3.. ^{+}Y2xxx
12	*d*	..2	*	*P*$4_3$32 *d*	4_3.. ^{+}Y3x$\bar{x}$
24	*e*	1	*	*P*$4_3$32 *e*	4_3.. ^{+}Y3x$\bar{x}$2yz

213 *P*$4_1$32

4	*a*	.32	*	*P*$4_3$32 *a*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ^{-}Y
4	*b*				^{-}Y
8	*c*	.3.	*	*P*$4_3$32 *c*	4_1.. ^{-}Y2xxx
12	*d*	..2	*	*P*$4_3$32 *d*	4_1.. ^{-}Y3x$\bar{x}$
24	*e*	1	*	*P*$4_3$32 *e*	4_1.. ^{-}Y3x$\bar{x}$2yz

214 *I*$4_1$32

8	*a*	.32	*	*I*$4_1$32 *a*	^{+}Y*
8	*b*				^{-}Y*
12	*c*	2.22	*	*I*$4_1$32 *c*	^{+}V
12	*d*				^{-}V
16	*e*	.3.	*	*I*$4_1$32 *e*	22.. *Y*2xxx

Table 3.4.3.3 (continued)

24	*f*	2..	*	$I4_132$ *f*	.3. *V*2*z*
24	*h*	..2	*	$I4_132$ *h*	4_3.. $^{+}Y^{*}3x\bar{x}$
24	*g*				4_1.. $^{-}Y^{*}3x\bar{x}$
48	*i*	1	*	$I4_132$ *i*	22.. $Y^{*}3x\bar{x}2yz$

215 $P\bar{4}3m$

1	*a*	$\bar{4}3m$		$Pm\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	$\bar{4}2.m$		$Pm\bar{3}m$ *c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
4	*e*	.3*m*	*	$P\bar{4}3m$ *e*	*P*4*xxx*
6	*f*	2.*mm*		$Pm\bar{3}m$ *e*	*P*6*z*
6	*g*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
12	*h*	2..		$Pm\bar{3}m$ *h*	.3. *J*4*x*
12	*i*	..*m*	*	$P\bar{4}3m$ *i*	*P*6*z*2*xx*
24	*j*	1	*	$P\bar{4}3m$ *j*	*P*6*z*2*xx*2*y*

216 $F\bar{4}3m$

4	*a*	$\bar{4}3m$		$Fm\bar{3}m$ *a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
4	*c*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*d*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
16	*e*	.3*m*	*	$F\bar{4}3m$ *e*	*F*4*xxx*
24	*f*	2.*mm*		$Fm\bar{3}m$ *e*	*F*6*z*
24	*g*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*6*z*
48	*h*	..*m*	*	$F\bar{4}3m$ *h*	*F*6*z*2*xx*
96	*i*	1	*	$F\bar{4}3m$ *i*	*F*6*z*2*xx*2*y*

217 $I\bar{4}3m$

2	*a*	$\bar{4}3m$		$Im\bar{3}m$ *a*	*I*
6	*b*	$\bar{4}2.m$		$Im\bar{3}m$ *b*	*J**
8	*c*	.3*m*	*	$I\bar{4}3m$ *c*	*I*4*xxx*
12	*d*	$\bar{4}$..		$Im\bar{3}m$ *d*	*W**
12	*e*	2.*mm*		$Im\bar{3}m$ *e*	*I*6*z*
24	*f*	2..		$Im\bar{3}m$ *g*	.3. *J**4*x*
24	*g*	..*m*	*	$I\bar{4}3m$ *g*	*I*6*z*2*xx*
48	*h*	1	*	$I\bar{4}3m$ *h*	*I*6*z*2*xx*2*y*

218 $P\bar{4}3n$

2	*a*	23.		$Im\bar{3}m$ *a*	*I*
6	*b*	222..		$Im\bar{3}m$ *b*	*J**
6	*c*	$\bar{4}$..		$Pm\bar{3}n$ *c*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *W*
6	*d*				*W*
8	*e*	.3.		$I\bar{4}3m$ *c*	*I*4*xxx*
12	*f*	2..		$Im\bar{3}m$ *e*	*I*6*z*
12	*g*	2..		$Pm\bar{3}n$ *g*	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *W*2*z*
12	*h*				.3. *W*2*z*
24	*i*	1	*	$P\bar{4}3n$ *i*	..*c* *I*6*z*2*xy*

219 $F\bar{4}3c$

8	*a*	23.		$Pm\bar{3}m$ *a*	P_2
8	*b*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*c*	$\bar{4}$..		$Pm\bar{3}m$ *c*	J_2
24	*d*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ J_2
32	*e*	.3.		$P\bar{4}3m$ *e*	$P_2$4*xxx*
48	*f*	2..		$Pm\bar{3}m$ *e*	$P_2$6*z*
48	*g*				$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $P_2$6*z*
96	*h*	1	*	$F\bar{4}3c$ *h*	..*n* $P_2$6*z*2*xy*

220 $I\bar{4}3d$

12	*a*	$\bar{4}$..	*	$I\bar{4}3d$ *a*	*S*
12	*b*				$'S$
16	*c*	.3.	*	$I\bar{4}3d$ *c*	$\bar{4}$.. $I_2Y^{**}1xxx$
24	*d*	2..	*	$I\bar{4}3d$ *d*	.3. *S*2*z*
48	*e*	1	*	$I\bar{4}3d$ *e*	.3*d* *S*4*xyz*

221 $Pm\bar{3}m$

1	*a*	$m\bar{3}m$	*	$Pm\bar{3}m$ *a*	*P*
1	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*
3	*c*	4/*mm.m*	*	$Pm\bar{3}m$ *c*	*J*
3	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *J*
6	*e*	4*m.m*	*	$Pm\bar{3}m$ *e*	*P*6*z*
6	*f*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*
8	*g*	.3*m*	*	$Pm\bar{3}m$ *g*	*P*8*xxx*
12	*h*	*mm*2..	*	$Pm\bar{3}m$ *h*	.3. *J*4*x*
12	*i*	*m.m*2	*	$Pm\bar{3}m$ *i*	*P*12*xx*
12	*j*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*12*xx*
24	*k*	*m*..	*	$Pm\bar{3}m$ *k*	*P*6*z*4*x*
24	*l*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*6*z*4*x*
24	*m*	..*m*	*	$Pm\bar{3}m$ *m*	*P*6*z*4*xx*
48	*n*	1	*	$Pm\bar{3}m$ *n*	*P*6*z*4*x*2*y*

222 $Pn\bar{3}n$

2	*a*	432		$Im\bar{3}m$ *a*	*I*
6	*b*	42.2		$Im\bar{3}m$ *b*	*J**
8	*c*	.$\bar{3}$.		$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	$\bar{4}$..		$Im\bar{3}m$ *d*	*W**
12	*e*	4..		$Im\bar{3}m$ *e*	*I*6*z*
16	*f*	.3.		$Im\bar{3}m$ *f*	*I*8*xxx*
24	*g*	2..		$Im\bar{3}m$ *g*	.3. *J**4*x*
24	*h*	..2		$Im\bar{3}m$ *h*	*I*12*xx*
48	*i*	1	*	$Pn\bar{3}n$ *i*	*n*.. *I*6*z*4*xy*

223 $Pm\bar{3}n$

2	*a*	$m\bar{3}$.		$Im\bar{3}m$ *a*	*I*
6	*b*	*mmm*..		$Im\bar{3}m$ *b*	*J**
6	*c*	$\bar{4}m.2$	*	$Pm\bar{3}n$ *c*	*W*
6	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *W*
8	*e*	.32		$Pm\bar{3}m$ *a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*f*	*mm*2..		$Im\bar{3}m$ *e*	*I*6*z*
12	*g*	*mm*2..	*	$Pm\bar{3}n$ *g*	.3. *W*2*z*
12	*h*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .3. *W*2*z*
16	*i*	.3.		$Im\bar{3}m$ *f*	*I*8*xxx*
24	*j*	..2	*	$Pm\bar{3}n$ *j*	.3. *W*4*xx*
24	*k*	*m*..	*	$Pm\bar{3}n$ *k*	..2 *I*6*z*2*x*
48	*l*	1	*	$Pm\bar{3}n$ *l*	..2 *I*6*z*2*x*2*y*

Table 3.4.3.3 (continued)

224 *Pn$\bar{3}$m*

2	*a*	$\bar{4}3m$		*Im$\bar{3}$m a*	*I*
4	*b*	$.\bar{3}m$		*Fm$\bar{3}$m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*
4	*c*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ *F*
6	*d*	$\bar{4}2.m$		*Im$\bar{3}$m b*	*J**
8	*e*	*.3m*	*	*Pn$\bar{3}$m e*	*..2 I4xxx*
12	*f*	2.22		*Im$\bar{3}$m d*	*W**
12	*g*	*2.mm*		*Im$\bar{3}$m e*	*I6z*
24	*h*	*2..*		*Im$\bar{3}$m g*	*.3. J***4x*
24	*i*	*..2*	*	*Pn$\bar{3}$m i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ $\bar{4}$*.. F6x$\bar{x}$*
24	*j*				$\frac{3}{4}\frac{3}{4}\frac{3}{4}$ $\bar{4}$*.. F6x$\bar{x}$*
24	*k*	*..m*	*	*Pn$\bar{3}$m k*	*..2 I6z2xx*
48	*l*	1	*	*Pn$\bar{3}$m l*	*..2 I6z2xx2y*

225 *Fm$\bar{3}$m*

4	*a*	*m$\bar{3}$m*	*	*Fm$\bar{3}$m a*	*F*
4	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F*
8	*c*	$\bar{4}3m$		*Pm$\bar{3}$m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
24	*d*	*m.mm*		*Pm$\bar{3}$m c*	J_2
24	*e*	*4m.m*	*	*Fm$\bar{3}$m e*	*F6z*
32	*f*	*.3m*	*	*Fm$\bar{3}$m f*	*F8xxx*
48	*g*	*2.mm*		*Pm$\bar{3}$m e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2*6z*
48	*h*	*m.m2*	*	*Fm$\bar{3}$m h*	*F12xx*
48	*i*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *F12xx*
96	*j*	*m..*	*	*Fm$\bar{3}$m j*	*F6z4x*
96	*k*	*..m*	*	*Fm$\bar{3}$m k*	*F6z4xx*
192	*l*	1	*	*Fm$\bar{3}$m l*	*F6z4x2y*

226 *Fm$\bar{3}$c*

8	*a*	432		*Pm$\bar{3}$m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
8	*b*	*m$\bar{3}$.*		*Pm$\bar{3}$m a*	P_2
24	*c*	$\bar{4}m.2$		*Pm$\bar{3}$m c*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ J_2
24	*d*	*4/m..*		*Pm$\bar{3}$m c*	J_2
48	*e*	*mm2..*		*Pm$\bar{3}$m e*	P_2*6z*
48	*f*	*4..*		*Pm$\bar{3}$m e*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2*6z*
64	*g*	*.3.*		*Pm$\bar{3}$m g*	P_2*8xxx*
96	*h*	*..2*		*Pm$\bar{3}$m i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2*12xx*
96	*i*	*m..*	*	*Fm$\bar{3}$c i*	*..2* P_2*6z2x*
192	*j*	1	*	*Fm$\bar{3}$c j*	*..2* P_2*6z2x2y*

227 *Fd$\bar{3}$m*

8	*a*	$\bar{4}3m$	*	*Fd$\bar{3}$m a*	*D*
8	*b*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *D*
16	*c*	*.$\bar{3}$m*	*	*Fd$\bar{3}$m c*	*T*
16	*d*				$\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *T*
32	*e*	*.3m*	*	*Fd$\bar{3}$m e*	*..2 D4xxx*
48	*f*	*2.mm*	*	*Fd$\bar{3}$m f*	*D6z*
96	*g*	*..m*	*	*Fd$\bar{3}$m g*	*..2 D6z2xx*
96	*h*	*..2*	*	*Fd$\bar{3}$m h*	$\bar{4}$*.. T6x$\bar{x}$*
192	*i*	1	*	*Fd$\bar{3}$m i*	*..2 D6z2xx2y*

228 *Fd$\bar{3}$c*

16	*a*	23.		*Im$\bar{3}$m a*	I_2
32	*b*	.32		*Fm$\bar{3}$m a*	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$ F_2
32	*c*	*.$\bar{3}$.*		*Fm$\bar{3}$m a*	$\frac{3}{8}\frac{3}{8}\frac{3}{8}$ F_2
48	*d*	$\bar{4}$*..*		*Im$\bar{3}$m b*	J^*_2
64	*e*	*.3.*		*Pn$\bar{3}$m e*	$(..2\ I4xxx)_2$
96	*f*	*2..*		*Im$\bar{3}$m e*	I_2*6z*
96	*g*	*..2*	*	*Fd$\bar{3}$c g*	$\frac{1}{8}\frac{1}{8}\frac{1}{8}$ $\bar{4}$*2.. F*$_2$*3x$\bar{x}$*
192	*h*	1	*	*Fd$\bar{3}$c h*	*d.2* I_2*6z2xy*

229 *Im$\bar{3}$m*

2	*a*	*m$\bar{3}$m*	*	*Im$\bar{3}$m a*	*I*
6	*b*	*4/mm.m*	*	*Im$\bar{3}$m b*	*J**
8	*c*	*.$\bar{3}$m*		*Pm$\bar{3}$m a*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2
12	*d*	$\bar{4}m.2$	*	*Im$\bar{3}$m d*	*W**
12	*e*	*4m.m*	*	*Im$\bar{3}$m e*	*I6z*
16	*f*	*.3m*	*	*Im$\bar{3}$m f*	*I8xxx*
24	*g*	*mm2..*	*	*Im$\bar{3}$m g*	*.3. J***4x*
24	*h*	*m.m2*	*	*Im$\bar{3}$m h*	*I12xx*
48	*i*	*..2*	*	*Im$\bar{3}$m i*	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *4..* P_2*6x$\bar{x}$*
48	*j*	*m..*	*	*Im$\bar{3}$m j*	*I6z4x*
48	*k*	*..m*	*	*Im$\bar{3}$m k*	*I6z4xx*
96	*l*	1	*	*Im$\bar{3}$m l*	*I6z4x2y*

230 *Ia$\bar{3}$d*

16	*a*	*.$\bar{3}$.*		*Im$\bar{3}$m a*	I_2
16	*b*	.32	*	*Ia$\bar{3}$d b*	*Y***
24	*c*	2.22	*	*Ia$\bar{3}$d c*	*V**
24	*d*	$\bar{4}$*..*	*	*Ia$\bar{3}$d d*	*S**
32	*e*	*.3.*	*	*Ia$\bar{3}$d e*	$\bar{4}$*..* *Y****2xxx*
48	*f*	*2..*	*	*Ia$\bar{3}$d f*	*.3. S***2z*
48	*g*	*..2*	*	*Ia$\bar{3}$d g*	$\bar{4}$*a..* *Y****3x$\bar{x}$*
96	*h*	1	*	*Ia$\bar{3}$d h*	$\bar{4}$*a..* I_2*6xyz*

crystal structures (Smirnova, 1962), of Patterson diagrams (Koch & Hellner, 1971), of Dirichlet domains (Koch, 1973, 1984) and of sphere packings for subperiodic groups (Koch & Fischer, 1978*b*).

The 30 lattice complexes in two-dimensional space correspond uniquely to the 'henomeric types of dot pattern' introduced by Grünbaum and Shephard (*cf. e.g.* Grünbaum & Shephard, 1981; Grünbaum, 1983).

3.4.4.2. Relations between crystal structures

Different crystal structures frequently show the same geometrical arrangement for some of their atoms, even though their space groups do not belong to the same type. In such cases, the corresponding Wyckoff positions either belong to the same lattice complex or there exists a close relationship between them, *e.g.* a limiting-complex relation.

Examples

(1) The Fe atoms in pyrite FeS_2 occupy Wyckoff position 4*a* .$\bar{3}$. 0, 0, 0 of $Pa\bar{3}$ (descriptive symbol *F*) that belongs to the invariant lattice complex $Fm\bar{3}m$ *a*. Accordingly, the Fe atoms in pyrite form a face-centred cubic lattice, as do the Cu atoms in the element structure of copper.

(2) Cuprite Cu_2O crystallizes with symmetry $Pn\bar{3}m$. The oxygen atoms occupy Wyckoff position 2*a* $\bar{4}3m$ 0, 0, 0 (descriptive symbol *I*) and the copper atoms position 4*b* .$\bar{3}m$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ (descriptive symbol $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ *F*). Position 2*a* belongs to lattice complex $Im\bar{3}m$ *a* and position 4*b* to $Fm\bar{3}m$ *a*. Therefore, the O atoms form a body-centred cubic lattice like the W atoms in the structure of tungsten, and the copper atoms form a face-centred cubic lattice. The tungsten configuration is shifted by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ with respect to the copper configuration.

(3) K_2NaAlF_6 (elpasolite, *cf.* Morss, 1974) and $K_2PbNi(NO_2)_6$ (*cf.* Takagi *et al.*, 1975) crystallize with symmetry $Fm\bar{3}m$ and $Fm\bar{3}$, respectively.

K_2NaAlF_6

Al	4*a*	$m\bar{3}m$	0, 0, 0	*F*
Na	4*b*	$m\bar{3}m$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	$\bar{4}3m$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
F	24*e*	4*m*.*m*	*x*, 0, 0	*F*6*z*
			$x = 0.219$	

$K_2PbNi(NO_2)_6$

Ni	4*a*	$m\bar{3}$.	0, 0, 0	*F*
Pb	4*b*	$m\bar{3}$.	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}F$
K	8*c*	23.	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$\frac{1}{4}\frac{1}{4}\frac{1}{4}P_2$
N	24*e*	*mm*2..	*x*, 0, 0	*F*6*z*
			$x = 0.1966$	
O	48*h*	*m*..	0, *y*, *z*	*F*6*z*2*x*

As the descriptive lattice-complex symbols for the various atomic positions show immediately, the two crystal structures are very similar. The only difference originates from the replacement of the fluorine atoms in elpasolite by NO_2 groups in $K_2PbNi(NO_2)_6$, which causes the symmetry reduction from $Fm\bar{3}m$ to $Fm\bar{3}$.

(4) The crystal structure of CoU (Baenziger *et al.*, 1950) may be interpreted as a slightly distorted CsCl (or β-brass, CuZn)-type structure. CsCl corresponds to Wyckoff positions 1*a* and 1*b* of $Pm\bar{3}m$ with descriptive symbols *P* and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ *P*, respectively; Co and U both occupy Wyckoff position 8*a* .3. *x*, *x*, *x* of $I2_13$ with $x = 0.0347$ for U and $x = 0.294$ for Co. As the descriptive symbol 2_12_1.. P_2Y^*1xxx shows, this Wyckoff position belongs to a Weissenberg complex with two invariant limiting complexes, namely *P* ($Pm\bar{3}m$ *a*) and Y^* ($I4_132$ *a*). $x = 0$ corresponds to P_2, $x = \frac{1}{4}$ to $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2, $x = \frac{1}{8}$ to $^+Y^*$ and $x = \frac{7}{8}$ to $^-Y^*$. Consequently, the uranium and cobalt atoms form approximately a P_2 and a $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ P_2 configuration, respectively.

Publications by Hellner (1965, 1976*a*,*b*,*c*, 1977, 1979), Loeb (1970), Smirnova & Vasserman (1971), Sakamoto & Takahasi (1971), Niggli (1971), Fischer & Koch (1974*b*), Hellner *et al.* (1981) and Hellner & Sowa (1985) refer to this aspect.

3.4.4.3. Reflection conditions

Wyckoff positions belonging to the same lattice complex show analogous reflection conditions. Therefore, lattice complexes have also been used to check the reflection conditions for all Wyckoff positions in the space-group tables of this volume.

Example

The lattice complex *oF* consists of all face-centred point lattices with orthorhombic symmetry. For its characteristic Wyckoff position *Fmmm* 4*a*, only the general conditions for reflections *hkl* in space group *Fmmm* are valid, namely $h + k$, $h + l$, $k + l = 2n$ (*cf.* Chapter 2.3). The non-characteristic Wyckoff position *Ccce* 4*a* also belongs to this lattice complex. The general reflection condition for *Ccce* is *hkl*: $h + k = 2n$. This has to be combined with $k + l = 2n$, the special condition for Wyckoff position *a*. Together the two conditions produce $h + l = 2n$, the third condition for a face-centred point lattice.

The descriptive symbols may supply information on the reflection conditions. If the symbol does not contain any distribution-symmetry part, the reflection conditions of the Wyckoff position are indicated by the symbol of the invariant lattice complex in the central part (*e.g.* *P*4/*nmm g*: *C*4*xx* shows that the reflection condition is that of a *C* lattice, *hkl*: $h + k = 2n$). In cases where the site set consists of only one point, *i.e.* the Wyckoff position belongs to a Weissenberg complex, all conditions for general reflections *hkl* that may arise from special choices of the coordinates can be read from the central part of the symbol (*e.g.* *P*4/*nmm c*: $0\frac{1}{2}0$ ..2 *CI*1*z* indicates that, by special choice of *z*, either *hkl*: $h + k = 2n$ or *hkl*: $h + k + l = 2n$ may be produced).

3.4.4.4. Phase transitions

If a crystal undergoes a phase transition from a high- to a low-symmetry modification, the transition may be connected with a group–subgroup transition. In such cases, the comparison of the lattice complexes corresponding to the Wyckoff positions of the original space group on the one hand and of its various subgroups on the other hand very often shows which of these subgroups are suitable for the low-symmetry modification.

This kind of procedure will be demonstrated with the aid of the space group $R\bar{3}m$ and its three *translationengleiche* subgroups with index 2, namely *R*32, $R\bar{3}$ and *R*3*m*. In the course of the restriction to a subgroup, the Wyckoff positions of $R\bar{3}m$ behave differently:

The descriptive symbols R and $00\frac{1}{2}\,R$ refer to Wyckoff positions $R\bar{3}m$ 3*a* and 3*b* as well as to Wyckoff positions $R32$ 3*a* and 3*b* and $R\bar{3}$ 3*a* and 3*b*. Therefore, all corresponding point configurations and atomic arrangements remain unchanged in these subgroups. In subgroup $R3m$, however, the respective Wyckoff position is 3*a* with descriptive symbol $R[z]$, *i.e.* a shift parallel to [001] of the entire point configuration is allowed.

The descriptive symbol $R2z$ for $R\bar{3}m$ 6*c* also occurs for $R32$ 6*c* and $R\bar{3}$ 6*c*. Again, neither subgroup allows any deformations of the corresponding point configurations or atomic arrangements. Symmetry reduction to $R3m$, however, yields a splitting of each $R2z$ configuration into two $R[z]$ configurations. The two z parameters may be chosen independently.

As M and $00\frac{1}{2}\,M$ are the descriptive symbols not only of $R\bar{3}m$ 9*e* and 9*d* but also of $R\bar{3}$ 9*e* and 9*d*, $R\bar{3}$ does not enable any deformation of the corresponding atomic arrangements. In $R32$ and in $R3m$, however, the respective point configurations may be differently deformed, as the descriptive symbols show: $R3x$ and $00\frac{1}{2}\,R3x$ ($R32$ 9*d* and 9*e*), $R3x\bar{x}[z]$ ($R3m$ 9*b*).

Wyckoff positions $R\bar{3}m$ 18*f* and 18*g* ($R6x$ and $00\frac{1}{2}\,R6x$) correspond to $R32$ 9*d* and 9*e* ($R3x$ and $00\frac{1}{2}\,R3x$), to $R\bar{3}$ 18*f* ($R6xyz$), and to $R3m$ 18*c* ($R3x\bar{x}2y[z]$). In $R32$, the hexagons $6x$ around the points of the R lattice are split into two oppositely oriented triangles $3x$, which may have different size. In $R\bar{3}$ and in $R3m$, the hexagons may be differently deformed.

Wyckoff position $R\bar{3}m$ 18*h* ($R6x\bar{x}z$) corresponds to sets of trigonal antiprisms around the points of an R lattice. These antiprisms may be distorted in $R32$ 18*f* ($R3x2yz$) or rotated in $R\bar{3}$ 18*f* ($R6xyz$). In $R3m$ 9*b* ($R3x\bar{x}[z]$), each antiprism is split into two parallel triangles that may differ in size.

In each of the three subgroups, any point configuration belonging to the general position $R\bar{3}m$ 36*i* splits into two parts. Each of these parts may be differently deformed.

3.4.4.5. Incorrect space-group assignment

In the literature, some crystal structures are still described within space groups that are only subgroups of the correct symmetry groups. Many such mistakes (but not all of them) could be avoided by simply looking at the lattice complexes (and their descriptive symbols) that correspond to the Wyckoff positions of the different kinds of atoms. Whenever the same (or an analogous) lattice-complex description of a crystal structure is also possible within a supergroup, then the crystal structure has at least that symmetry.

Examples

(1) The crystal structure of β-$LiRhO_2$ has been refined in space group $F4_132$ (*cf.* Hobbie & Hoppe, 1986).

Rh	16*c*	.32	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	T
Li	16*d*	.32	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\,T$
O	32*e*	.3.	x,x,x	..2 $D4xxx$

The same atomic arrangement is possible in the supergroup $Fd\bar{3}m$ of $F4_132$, as can easily be read from Table 3.4.3.3:

Rh	16*c*	$.\bar{3}m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	T
Li	16*d*	$.\bar{3}m$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{1}{2}\frac{1}{2}\frac{1}{2}\,T$
O	32*e*	.3*m*	x,x,x	..2 $D4xxx$

Therefore, β-$LiRhO_2$ should be described in $Fd\bar{3}m$.

(2) $KIAs_4O_6$ (Pertlik, 1988) has been described with symmetry $P622$.

I	1*a*	622	$0,0,0$	P
K	1*b*	622	$0,0,\frac{1}{2}$	$00\frac{1}{2}\,P$
As	4*h*	3..	$\frac{1}{3},\frac{2}{3},z$	$G2z$
O	6*i*	2..	$\frac{1}{2},0,z$	$N2z$

Space group $P6/mmm$ allows the same atomic arrangement:

I	1*a*	$6/mmm$	$0,0,0$	P
K	1*b*	$6/mmm$	$0,0,\frac{1}{2}$	$00\frac{1}{2}\,P$
As	4*h*	3*m*.	$\frac{1}{3},\frac{2}{3},z$	$G2z$
O	6*i*	2*mm*	$\frac{1}{2},0,z$	$N2z$

Therefore, $KIAs_4O_6$ should be described in $P6/mmm$.

3.4.4.6. Application of descriptive lattice-complex symbols

Descriptive symbols of lattice complexes – at least those of the invariant lattice complexes – have been used for the description of crystal structures (*cf.* Section 3.4.4.2 and the literature cited there), for the nomenclature of three-periodic surfaces (von Schnering & Nesper, 1987) and in connection with orbifolds of space groups (Johnson *et al.*, 2001).

3.4.4.7. Weissenberg complexes

In general, each lattice complex involves point configurations that cannot be related to any crystal structure because the shortest distances between the atoms in a corresponding arrangement would become too small. Only the 67 Weissenberg complexes (*cf.* Section 3.4.1.5.2) form an exception from this rule. Assuming that the metrical parameters are chosen adequately, each point configuration stemming from a Weissenberg complex may, in principle, refer to the arrangement of some atoms in a crystal structure. In case of the 36 invariant lattice complexes this property is immediately evident. The further 31 Weissenberg complexes have one or more degrees of freedom (*cf.* Section 3.4.1.5.2 and Table 3.4.1.1). Nevertheless, varying the corresponding free coordinate parameters never results in point configurations with infinitesimally small distances.

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3.5. Normalizers of space groups and their use in crystallography

E. Koch, W. Fischer and U. Müller

3.5.1. Introduction and definitions

By E. Koch, W. Fischer and U. Müller

3.5.1.1. Introduction

The mathematical concept of normalizers forms the common basis for the solution of several crystallographic problems:

It is generally known, for instance, that the coordinate description of a crystal structure trivially depends on the coordinate system used for the description, *i.e.* on the setting of the space group and the site symmetry of the origin. It is less well known, however, that for most crystal structures there exist several different but equivalent coordinate descriptions, even if the space-group setting and the site symmetry of the origin are unchanged. The number of such descriptions varies between 1 and 24 and depends only on the type of the Euclidean normalizer of the corresponding space group. In principle, none of these descriptions stands out against the others.

In crystal-structure determination with direct methods, the phases of some suitably chosen structure factors have to be restricted to certain values or to certain ranges in order to specify the origin and the enantiomorph. The information necessary for a correct selection of such phases and for their appropriate restrictions follows directly from the Euclidean normalizer of the space group. Similar examples are the positioning of the first atom(s) within an asymmetric unit when using trial-and-error or Patterson methods, the choice of a basis system for indexing the reflections of a diffraction pattern or the indexing of the first morphological face(s) of a crystal.

For the following problems, normalizers also play an important role: They supply information on the interchangeability of Wyckoff positions and their assignment to Wyckoff sets (*cf.* Section 1.4.4 and Chapter 3.4), needed *e.g.* for the definition of lattice complexes. They are important for the comparison of crystal structures, for their assignment to structure types and for the choice of a standard description for each crystal structure (Parthé & Gelato, 1984, 1985). They allow the derivation of 'privileged origins' for each space group (Burzlaff & Zimmermann, 1980) and facilitate the complete deduction of subgroups and supergroups of a crystallographic group. They enable an easy classification of magnetic (black–white or Shubnikov) space groups and of colour space groups. They may also be used to reduce the parameter range in the study of geometrical properties of point configurations, *e.g.* their eigensymmetry or their sphere packings and Dirichlet partitions (*cf. e.g.* Koch, 1984*a*).

In the past, most of these problems have been treated by crystallographers without the aid of normalizers, but the use of normalizers simplifies the solution of all these problems and clarifies the common background (for references, see Fischer & Koch, 1983).

3.5.1.2. Definitions

Any pair, consisting of a group $\mathcal{G}$ and one of its supergroups $\mathcal{S}$, is uniquely related to a third intermediate group $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$, called the *normalizer of* $\mathcal{G}$ *with respect to* $\mathcal{S}$. $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$ is defined as the set of all elements $s \in \mathcal{S}$ that map $\mathcal{G}$ onto itself by conjugation (*cf.* Section 1.1.8):

$$\mathcal{N}_{\mathcal{S}}(\mathcal{G}) := \{s \in \mathcal{S} \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

The normalizer $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$ may coincide either with $\mathcal{G}$ or with $\mathcal{S}$ or it may be a proper intermediate group. In any case, $\mathcal{G}$ is a normal subgroup of its normalizer.

For most crystallographic problems, three kinds of normalizers are of special interest:

(i) The normalizer of a space group (plane group) $\mathcal{G}$ with respect to the group $\mathcal{E}$ of all Euclidean mappings (motions, isometries) in $\mathbb{E}^3$ ($\mathbb{E}^2$), called the *Euclidean normalizer of* $\mathcal{G}$:

$$\mathcal{N}_{\mathcal{E}}(\mathcal{G}) := \{s \in \mathcal{E} \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

(ii) The normalizer of a space group (plane group) $\mathcal{G}$ with respect to the group $\mathcal{A}$ of all affine mappings in $\mathbb{E}^3$ ($\mathbb{E}^2$), called the *affine normalizer of* $\mathcal{G}$:

$$\mathcal{N}_{\mathcal{A}}(\mathcal{G}) := \{s \in \mathcal{A} \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

(iii) The normalizer of a space group $\mathcal{G}$ with respect to the group $\mathcal{E}^+$ of all chirality-preserving Euclidean mappings in $\mathbb{E}^3$, *i.e.* of all translations and proper rotations (including screw rotations), but excluding symmetry operations of the second kind (*viz.* inversions, reflections, glide reflections and rotoinversions). We call it the *chirality-preserving Euclidean normalizer of* $\mathcal{G}$:

$$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}) := \{s \in \mathcal{E}^+ \mid s^{-1}\mathcal{G}s = \mathcal{G}\}.$$

$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ exists only if $\mathcal{G}$ is a Sohncke space group. The 65 *Sohncke space-group types* are those space-group types that have no symmetry operations of the second kind (Flack, 2003).[1] They include the eleven pairs of types of enantiomorphic space groups; these eleven pairs are the only ones where the space groups themselves are chiral, *i.e.* which have an Euclidean normalizer containing only isometries of the first kind. The space groups of the remaining 43 Sohncke types are not chiral but do allow chiral crystal structures. A rigid object (or spatial arrangement of points or atoms) is *chiral* if it is nonsuperposable by pure rotation or translation on its image formed by inversion through a point. A chiral crystal structure is compatible only with a Sohncke space group.

The Euclidean normalizers of the space groups were first derived by Hirshfeld (1968) under the name *Cheshire groups*. They have been tabulated in more detail by Gubler (1982*a*,*b*) and Fischer & Koch (1983). The Euclidean normalizers of triclinic and monoclinic space groups with specialized metric of the lattice were determined by Koch & Müller (1990). The affine normalizers of the space groups have been listed by Burzlaff & Zimmermann (1980), Billiet *et al.* (1982) and Gubler (1982*a*,*b*). They were also used for the derivation of Wyckoff sets and the

[1] Sohncke (1879) was the first to derive the 65 space-group types having only symmetry operations of the first kind (translations, rotations and screw rotations). As proposed by Flack (2003), these are called the 65 Sohncke space-group types.

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definition of lattice complexes by Koch & Fischer (1975), even though there the automorphism groups of the space groups were tabulated instead of their affine normalizers. The chirality-preserving Euclidean normalizers are tabulated in this volume for the first time.

3.5.2. Euclidean and affine normalizers of plane groups and space groups

By E. Koch, W. Fischer and U. Müller

3.5.2.1. Euclidean normalizers of plane groups and space groups

Since each symmetry operation of the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ maps the space group $\mathcal{G}$ onto itself, it also maps the set of all symmetry elements of $\mathcal{G}$ onto itself. Therefore, the Euclidean normalizer of a space group can be interpreted as the group of motions that maps the pattern of symmetry elements of the space group onto itself, *i.e.* as the 'symmetry of the symmetry pattern'.

For most space (plane) groups, the Euclidean normalizers are space (plane) groups again. Exceptions are those groups where origins are not fully fixed by symmetry, *i.e.* all space groups of the geometrical crystal classes 1, *m*, 2, 2*mm*, 3, 3*m*, 4, 4*mm*, 6 and 6*mm*, and all plane groups of the geometrical crystal classes 1 and *m*. The Euclidean normalizer of each such group contains continuous translations (*i.e.* translations of infinitesimal length) in one, two or three independent lattice directions and, therefore, is not a space (plane) group but a supergroup of a space (plane) group.

If one regards a certain type of space (plane) group, usually the Euclidean normalizers of all corresponding groups belong also to only one type of normalizer. This is true for all cubic, hexagonal, trigonal and tetragonal space groups (hexagonal and square plane groups) and, in addition, for 21 types of orthorhombic space group (4 types of rectangular plane group), *e.g.* for *Pnma*.

In contrast to this, the Euclidean normalizer of a space (plane) group belonging to one of the other 38 orthorhombic (3 rectangular) types may interchange two or even three lattice directions if the corresponding basis vectors have equal length (example: *Pmmm* with $a = b$). Then, the Euclidean normalizer of this group belongs to the tetragonal (square) or even to the cubic crystal system, whereas another space (plane) group of the same type but with general metric has an orthorhombic (rectangular) Euclidean normalizer.

For each space (plane)-group type belonging to the monoclinic (oblique) or triclinic system, there also exist groups with specialized metric that have Euclidean normalizers of higher symmetry than for the general case (*cf.* Koch & Müller, 1990). The description of these special cases, however, is by far more complicated than for the orthorhombic system.

The symmetry of the Euclidean normalizer of a monoclinic (oblique) space (plane) group depends only on two metrical parameters. A clear presentation of all cases with specialized metric may be achieved by choosing the cosine of the monoclinic angle and the related axial ratio as parameters. To cover all different metrical situations exactly once, not all pairs of parameter values are allowed for a given type of space (plane) group, but one has to restrict the study to a certain parameter range depending on the type, the setting and the cell choice of the space (plane) group. Parthé & Gelato (1985) have discussed in detail such parameter regions for the first setting of the monoclinic space groups. Figs. 3.5.2.1 to 3.5.2.4 are based on these studies.

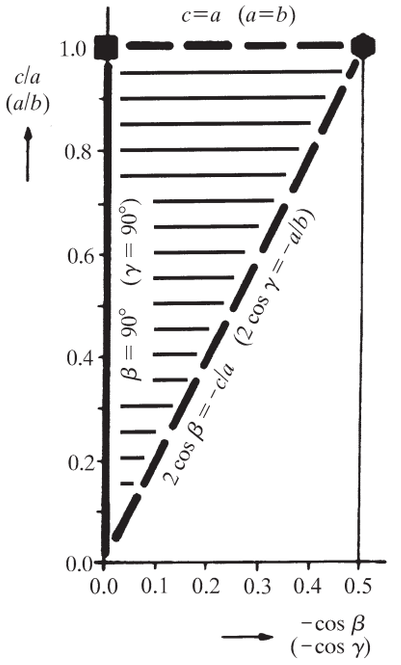

Figure 3.5.2.1
Parameter range for space groups of types $P2$, $P2_1$, Pm, $P2/m$ and $P2_1/m$ (plane groups of types $p1$ and $p2$). The information in parentheses refers to unique axis *c*.

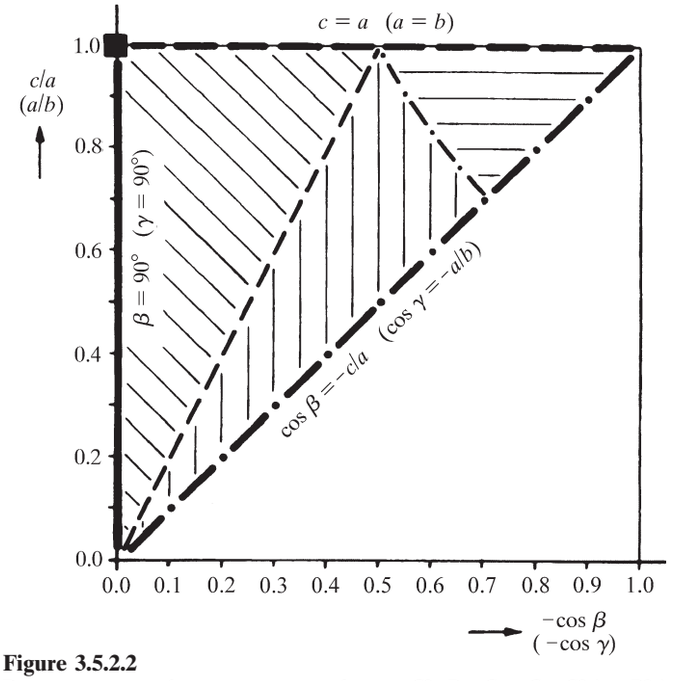

Figure 3.5.2.2
Parameter range for space groups of types $C2$, Pc, Cm, Cc, $C2/m$, $P2/c$, $P2_1/c$ and $C2/c$. They refer to the following settings:
unique axis *b*, cell choice 2: $P1n1$, $P12/n1$, $P12_1/n1$;
unique axis *b*, cell choice 3: $I121$, $I1m1$, $I1a1$, $I12/m1$, $I12/a1$;
unique axis *c*, cell choice 2: $P11n$, $P112/n$, $P112_1/n$;
unique axis *c*, cell choice 3: $I112$, $I11m$, $I11b$, $I112/m$, $I112/b$.
The information in parentheses refers to unique axis *c*.

Fig. 3.5.2.1 shows a suitably chosen parameter region for the five space-group types $P2$, $P2_1$, Pm, $P2/m$ and $P2_1/m$ and for the plane-group types $p1$ and $p2$. Each such space (plane) group with general metric may be uniquely assigned to an inner point of this region and any metrical specialization corresponds either to one of the three boundary lines or to one of their points of inter-

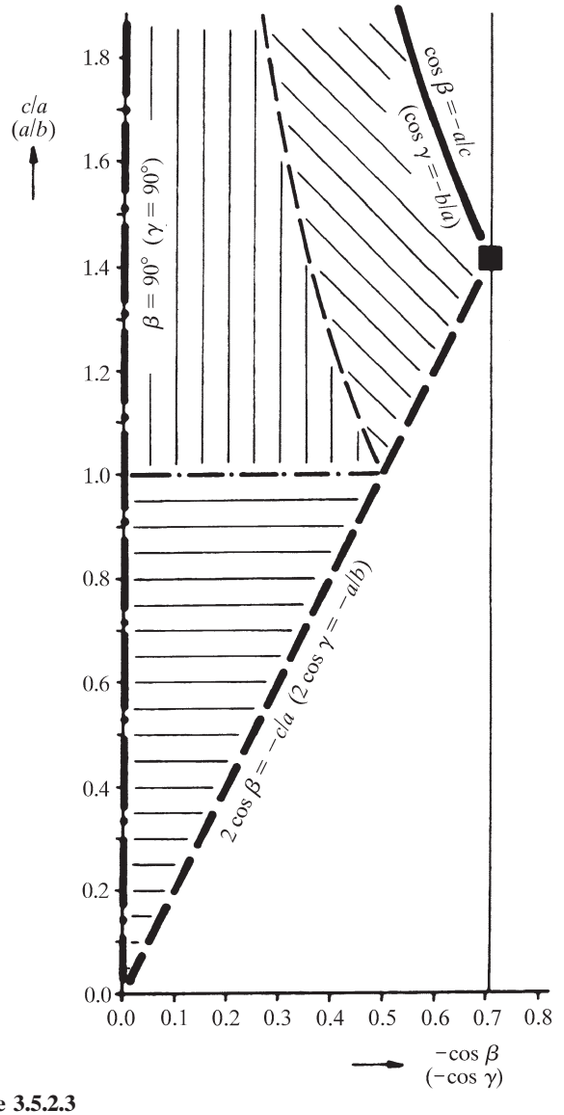

Figure 3.5.2.3
Parameter range for space groups of types *C*2, *Pc*, *Cm*, *Cc*, *C*2/*m*, *P*2/*c*, $P2_1/c$ and *C*2/*c*:
unique axis *b*, cell choice 1: *P*1*c*1, *P*12/*c*1, $P12_1/c1$;
unique axis *b*, cell choice 2: *A*121, *A*1*m*1, *A*1*n*1, *A*12/*m*1, *A*12/*n*1;
unique axis *c*, cell choice 1: *P*11*a*, *P*112/*a*, $P112_1/a$;
unique axis *c*, cell choice 2: *B*112, *B*11*m*, *B*11*n*, *B*112/*m*, *B*112/*n*.
The information in parentheses refers to unique axis *c*.

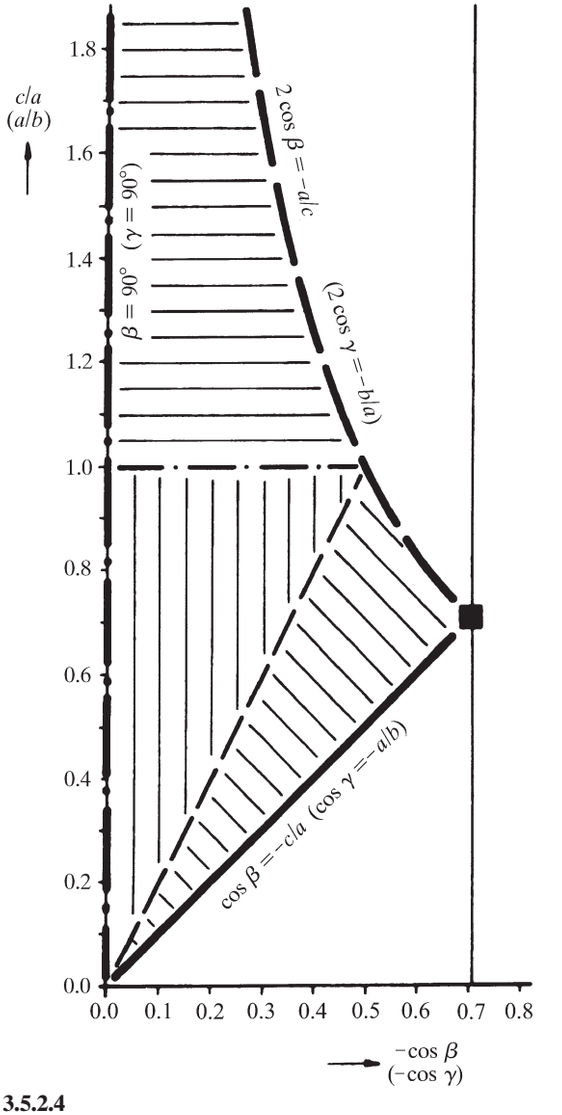

Figure 3.5.2.4
Parameter range for space groups of types *C*2, *Pc*, *Cm*, *Cc*, *C*2/*m*, *P*2/*c*, $P2_1/c$ and *C*2/*c*:
unique axis *b*, cell choice 1: *C*121, *C*1*m*1, *C*1*c*1, *C*12/*m*1, *C*12/*c*1;
unique axis *b*, cell choice 3: *P*1*a*1, *P*12/*a*1, $P12_1/a1$, *C*12/*c*1;
unique axis *c*, cell choice 1: *A*112, *A*11*m*, *A*11*a*, *A*112/*m*, *A*112/*a*;
unique axis *c*, cell choice 3: *P*11*b*, *P*112/*b*, $P112_1/b$, *A*112/*a*.
The information in parentheses refers to unique axis *c*.

section and gives rise to a symmetry enhancement of the respective Euclidean normalizer.

For each of the other eight types of monoclinic space groups, *i.e.* *C*2, *Pc*, *Cm*, *Cc*, *C*2/*m*, *P*2/*c*, $P2_1/c$ and *C*2/*c*, and for each setting three possibilities of cell choice are listed in Chapter 2.3, which can be distinguished by different space-group symbols (example: *C*12/*m*1, *A*12/*m*1, *I*12/*m*1, *A*112/*m*, *B*112/*m*, *I*112/*m*). For each setting, there exist two ways to choose a suitable range for the metrical parameters such that each group corresponds to exactly one point:

(i) One arbitrarily restricts oneself to cell choice 1, 2 or 3. Then, the suitable parameter range (displayed in one of the Figs. 3.5.2.2, 3.5.2.3 or 3.5.2.4) is larger than the range shown in Fig. 3.5.2.1 because, in contrast to the space-group types discussed above, some of the possible metrical specializations do not give rise to any symmetry enhancement of the Euclidean normalizers. These special metrical cases refer to the light lines subdividing the parameter regions of Figs. 3.5.2.2 to 3.5.2.4. Again, all inner points of these regions correspond to space groups with Euclidean normalizers without enhanced symmetry, and all points on the heavy-line boundaries refer to space groups, the Euclidean normalizers of which show symmetry enhancement.

(ii) For all types of monoclinic space groups, one regards only the small parameter region shown in Fig. 3.5.2.1, but in return takes into consideration all three possibilities for the cell choice. Then, however, not all boundaries of this small parameter region correspond to Euclidean normalizers with enhanced symmetry. (Similar considerations are true for oblique plane groups.)

For triclinic space groups, five metrical parameters are necessary and, therefore, it is impossible to describe the special metrical cases in an analogous way.

In general, between a space group (or plane group) $\mathcal{G}$ and its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, two uniquely defined intermediate groups $\mathcal{K}(\mathcal{G})$ and $\mathcal{L}(\mathcal{G})$ exist, such that

Table 3.5.2.1
Euclidean normalizers of the plane groups

For the restrictions of the cell metric of the two oblique plane groups see text and Fig. 3.5.2.3.

Plane group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G})$		Additional generators of $\mathcal{N}_\mathcal{E}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Twofold rotation	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$
1	$p1$	General	$p^2 2$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}$	$r, 0;\ 0, s$	$-x, -y$		$\infty^2 \cdot 2 \cdot 1$
		$a < b,\ \gamma = 90°$	$p^2 2mm$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}$	$r, 0;\ 0, s$	$-x, -y$	$-x,\ y$	$\infty^2 \cdot 2 \cdot 2$
		$2\cos\gamma = -a/b,\ 90° < \gamma < 120°$	$c^2 2mm$	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b})$	$r, 0;\ 0, s$	$-x, -y$	$x-y, -y$	$\infty^2 \cdot 2 \cdot 2$
		$a = b,\ 90° < \gamma < 120°$	$c^2 2mm$	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b})$	$r, 0;\ 0, s$	$-x, -y$	y, x	$\infty^2 \cdot 2 \cdot 2$
		$a = b,\ \gamma = 90°$	$p^2 4mm$	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}$	$r, 0;\ 0, s$	$-x, -y$	$-x,\ y;\ y,\ x$	$\infty^2 \cdot 2 \cdot 4$
		$a = b,\ \gamma = 120°$	$p^2 6mm$	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}$	$r, 0;\ 0, s$	$-x, -y$	$y,\ x;\ x,\ x-y$	$\infty^2 \cdot 2 \cdot 6$
2	$p2$	General	$p2$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a < b,\ \gamma = 90°$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$		$-x,\ y$	$4 \cdot 1 \cdot 2$
		$2\cos\gamma = -a/b,\ 90° < \gamma < 120°$	$c2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$		$x-y, -y$	$4 \cdot 1 \cdot 2$
		$a = b,\ 90° < \gamma < 120°$	$c2mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$		$y,\ x$	$4 \cdot 1 \cdot 2$
		$a = b,\ \gamma = 90°$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$		$-x,\ y;\ y,\ x$	$4 \cdot 1 \cdot 4$
		$a = b,\ \gamma = 120°$	$p6mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$		$y,\ x;\ x,\ x-y$	$4 \cdot 1 \cdot 6$
3	$p1m1$		$p^1 2mm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2}, 0;\ 0, s$	$-x, -y$		$(2 \cdot \infty) \cdot 2 \cdot 1$
4	$p1g1$		$p^1 2mm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2}, 0;\ 0, s$	$-x, -y$		$(2 \cdot \infty) \cdot 2 \cdot 1$
5	$c1m1$		$p^1 2mm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$0, s$	$-x, -y$		$\infty \cdot 2 \cdot 1$
6	$p2mm$	$a \neq b$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$		y, x	$4 \cdot 1 \cdot 2$
7	$p2mg$		$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
8	$p2gg$	$a \neq b$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$			$4 \cdot 1 \cdot 1$
		$a = b$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0;\ 0, \frac{1}{2}$		y, x	$4 \cdot 1 \cdot 2$
9	$c2mm$	$a \neq b$	$p2mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0$			$2 \cdot 1 \cdot 1$
		$a = b$	$p4mm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0$		y, x	$2 \cdot 1 \cdot 2$
10	$p4$		$p4mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$		y, x	$2 \cdot 1 \cdot 2$
11	$p4mm$		$p4mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
12	$p4gm$		$p4mm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b})$	$\frac{1}{2}, \frac{1}{2}$			$2 \cdot 1 \cdot 1$
13	$p3$		$p6mm$	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}), \frac{1}{3}(-\mathbf{a}+\mathbf{b})$	$\frac{2}{3}, \frac{1}{3}$	$-x, -y$	y, x	$3 \cdot 2 \cdot 2$
14	$p3m1$		$p6mm$	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}), \frac{1}{3}(-\mathbf{a}+\mathbf{b})$	$\frac{2}{3}, \frac{1}{3}$	$-x, -y$		$3 \cdot 2 \cdot 1$
15	$p31m$		$p6mm$	$\mathbf{a}, \mathbf{b}$		$-x, -y$		$1 \cdot 2 \cdot 1$
16	$p6$		$p6mm$	$\mathbf{a}, \mathbf{b}$			y, x	$1 \cdot 1 \cdot 2$
17	$p6mm$		$p6mm$	$\mathbf{a}, \mathbf{b}$				$1 \cdot 1 \cdot 1$

$$\mathcal{G} \leq \mathcal{K}(\mathcal{G}) \leq \mathcal{L}(\mathcal{G}) \leq \mathcal{N}_\mathcal{E}(\mathcal{G})$$

holds. $\mathcal{K}(\mathcal{G})$ is that *klassengleiche* supergroup of $\mathcal{G}$ that is at the same time a *translationengleiche* subgroup of $\mathcal{N}_\mathcal{E}(\mathcal{G})$. It is well defined according to the theorem of Hermann (1929). The group $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$ only if $\mathcal{G}$ is noncentrosymmetric but $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is centrosymmetric; then $\mathcal{L}(\mathcal{G})$ is that centrosymmetric supergroup of $\mathcal{K}(\mathcal{G})$ of index 2 that is again a subgroup of $\mathcal{N}_\mathcal{E}(\mathcal{G})$. It belongs to the Laue class of $\mathcal{G}$. If $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is noncentrosymmetric, an intermediate group $\mathcal{L}(\mathcal{G})$ cannot exist.

The chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ of a Sohncke space group $\mathcal{G}$ is the unique noncentrosymmetric subgroup of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ which is a supergroup of $\mathcal{K}(\mathcal{G})$:

$$\mathcal{G} \leq \mathcal{K}(\mathcal{G}) \leq \mathcal{N}_{\mathcal{E}^+}(\mathcal{G}) \leq \mathcal{N}_\mathcal{E}(\mathcal{G}).$$

If $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is centrosymmetric, $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is a subgroup of index 2 of $\mathcal{N}_\mathcal{E}(\mathcal{G})$. If $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is noncentrosymmetric, $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ and $\mathcal{N}_\mathcal{E}(\mathcal{G})$ are identical.

With the aid of its chirality-preserving Euclidean normalizer it is possible to determine all equivalent sets of coordinates of a chiral crystal structure, excluding the opposite enantiomorph (*cf.* Section 3.5.3.2).

The groups $\mathcal{K}(\mathcal{G})$ and $\mathcal{L}(\mathcal{G})$ are of special interest in connection with direct methods for structure determination: they cause the parity classes of reflections; $\mathcal{K}(\mathcal{G})$ defines the permissible origin shifts and the parameter ranges for the phase restrictions in the specification of the origin; and $\mathcal{L}(\mathcal{G})$ gives information on possible phase restrictions for the selection of the enantiomorph. For any space (plane) group $\mathcal{G}$, the translation subgroups of $\mathcal{K}(\mathcal{G})$, $\mathcal{L}(\mathcal{G})$, $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and even $\mathcal{N}_\mathcal{A}(\mathcal{G})$ coincide.

The Euclidean normalizers of the plane groups are listed in Table 3.5.2.1, those of triclinic space groups in Table 3.5.2.2. The Euclidean and the chirality-preserving Euclidean normalizers of monoclinic and orthorhombic space groups are in Tables 3.5.2.3 and 3.5.2.4, those of all other space groups in Table 3.5.2.5. Herein all settings and choices of cell and origin as tabulated in Chapters 2.2 and 2.3 are taken into account and, in addition, all metrical specializations giving rise to Euclidean normalizers with enhanced symmetry. Each setting, cell choice, origin or metrical specialization corresponds to one line in the tables. (Exceptions are some orthorhombic space groups with tetragonal metric: if $a = b$ as well as $b = c$ and $c = a$ give rise to a symmetry enhancement of the Euclidean normalizer, only the case $a = b$ is listed in Table 3.5.2.4.)

The first column of Tables 3.5.2.1, 3.5.2.3, 3.5.2.4 and 3.5.2.5 shows the number of the plane group or space group, and the second column shows its Hermann–Mauguin symbol together with information on the setting, cell choice and origin, if neces-

Table 3.5.2.2
Euclidean normalizers of the triclinic space groups

Basis vectors of the Euclidean normalizers ($\mathbf{a}_c$, $\mathbf{b}_c$, $\mathbf{c}_c$ refer to the possibly centred conventional unit cell for the respective Bravais lattice): $P1$: $\varepsilon\mathbf{a}_c, \varepsilon\mathbf{b}_c, \varepsilon\mathbf{c}_c$; $P\bar{1}$: $\frac{1}{2}\mathbf{a}_c, \frac{1}{2}\mathbf{b}_c, \frac{1}{2}\mathbf{c}_c$.

	Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G})$ of	
Bravais type	$P1$ (1)	$P\bar{1}$ (2)
aP	$P^3\bar{1}$	$P\bar{1}$
mP	P^32/m	$P2/m$
mA	P^32/m	$A2/m$
oP	P^3mmm	$Pmmm$
oC	P^3mmm	$Cmmm$
oF	P^3mmm	$Fmmm$
oI	P^3mmm	$Immm$
tP	P^34/mmm	$P4/mmm$
tI	P^34/mmm	$I4/mmm$
hP	P^36/mmm	$P6/mmm$
hR	$P^3\bar{3}m1$	$R\bar{3}m$
cP	$P^3m\bar{3}m$	$Pm\bar{3}m$
cF	$P^3m\bar{3}m$	$Fm\bar{3}m$
cI	$P^3m\bar{3}m$	$Im\bar{3}m$

sary. Special metrical conditions affecting the Euclidean normalizer are tabulated in the third column of Tables 3.5.2.1, 3.5.2.3 and 3.5.2.4. The term 'general' means that only the general metrical conditions for the respective crystal system are valid. In Table 3.5.2.5, a corresponding column is superfluous because here a metrical specialization of the space group does not influence the type of the Euclidean normalizer.

The Euclidean normalizer of the space (plane) group is identified in the fourth column of Tables 3.5.2.3 and 3.5.2.4 (3.5.2.1) or in the third column of Table 3.5.2.5. As Euclidean normalizers are groups of motions, they can normally be designated by Hermann–Mauguin symbols. If, however, the origin of the space (plane) group is not fixed by symmetry (examples: $P4$, $P1m1$, $P1$), the Euclidean normalizer contains continuous translations in one, two or three (one or two) independent directions. In these cases, P^1, B^1, C^1, P^2 or P^3 (p^1, c^1, p^2), respectively, are used instead of the Bravais letter.[2] The setting and origin choice for the Euclidean normalizers are indicated as for space groups. In a few cases, origin choices not tabulated in Chapter 2.3 or nonconventional settings like *Bmmm* instead of *Cmmm* are needed.

In the next column, the basis of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is described in terms of the basis of $\mathcal{G}$. A factor ε is used to indicate continuous translations.

The following three columns specify the set of additional symmetry operations that generate $\mathcal{K}(\mathcal{G})$, $\mathcal{L}(\mathcal{G})$ and $\mathcal{N}_\mathcal{E}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ successively from the space group $\mathcal{G}$. The first of them shows the vector components of the additional translations generating $\mathcal{K}(\mathcal{G})$ from $\mathcal{G}$; components referring to continuous translations are labelled r, s and t. If $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$, *i.e.* if $\mathcal{G}$ is noncentrosymmetric and $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is centrosymmetric, the position of the additional centre of inversion is given in the second of these columns. The respective inversion generates $\mathcal{L}(\mathcal{G})$ from $\mathcal{K}(\mathcal{G})$. (For plane groups, additional twofold rotations play the role of these inversions.) $\mathcal{L}(\mathcal{G})$, however, is undefined for $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ and also if $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is noncentrosymmetric; this fact is indicated by a slash. The last of these columns contains entries only if $\mathcal{G}$ belongs to a different Laue class than $\mathcal{N}_\mathcal{E}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$. The corresponding additional generators are listed as coordinate triplets.

In the last column, the subgroup index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is specified as the product $k_g l_k n_l$, where k_g means the index of $\mathcal{G}$ in $\mathcal{K}(\mathcal{G})$, l_k the index of $\mathcal{K}(\mathcal{G})$ in $\mathcal{L}(\mathcal{G})$ and n_l the index of $\mathcal{L}(\mathcal{G})$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$. [In the case of a noncentrosymmetric normalizer, the index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ is given as the product $k_g n_k$, where k_g means the index of $\mathcal{G}$ in $\mathcal{K}(\mathcal{G})$ and n_k the index of $\mathcal{K}(\mathcal{G})$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$.] For continuous translations, k_g is always infinite. Nevertheless, it is useful to distinguish different cases: ∞, ∞^2 and ∞^3 refer to one, two and three independent directions with continuous translations. An additional factor of 2^n or 3^n indicates the existence of n additional independent translations which are not continuous.

For triclinic space groups, each metrical specialization gives rise to a symmetry enhancement of the Euclidean normalizer. The corresponding conditions for the metrical parameters, however, cannot be described as easily as in the monoclinic case (for further information see Chapter 3.1 and the literature on 'reduced cells' cited therein). Table 3.5.2.2 shows the Euclidean normalizers for $P1$ and $P\bar{1}$. Each special metrical condition is designated by the Bravais type of the corresponding translation lattice. In the case of $P\bar{1}$, the Euclidean normalizer is always the eigensymmetry group of a suitably chosen point lattice with basis vectors $\frac{1}{2}\mathbf{a}_c$, $\frac{1}{2}\mathbf{b}_c$ and $\frac{1}{2}\mathbf{c}_c$. Here, $\mathbf{a}_c$, $\mathbf{b}_c$ and $\mathbf{c}_c$ do not refer to the primitive unit cell of $P\bar{1}$ but to the possibly centred conventional cell for the respective Bravais lattice. In the case of $P1$, the Euclidean normalizer always contains continuous translations in three independent directions, symbolized by P^3. These normalizers may be easily derived from those for $P\bar{1}$.

3.5.2.2. Affine normalizers of plane groups and space groups

The affine normalizer $\mathcal{N}_\mathcal{A}(\mathcal{G})$ of a space (plane) group $\mathcal{G}$ either is a true supergroup of its Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G})$, or both normalizers coincide:

$$\mathcal{N}_\mathcal{A}(\mathcal{G}) \geq \mathcal{N}_\mathcal{E}(\mathcal{G}).$$

As any translation is an isometry, each translation belonging to $\mathcal{N}_\mathcal{A}(\mathcal{G})$ also belongs to $\mathcal{N}_\mathcal{E}(\mathcal{G})$. Therefore, the affine normalizer and the Euclidean normalizer of a space (plane) group necessarily have identical translation subgroups.

By analogy to the isometries of the Euclidean normalizer, the additional mappings of the affine normalizer also map the set of all symmetry elements of the space (plane) group onto itself.

In contrast to the Euclidean normalizers, the affine normalizers of all space (plane) groups of a certain type belong to only one type of normalizer, *i.e.* they are isomorphic groups. Therefore, the type of the affine normalizer $\mathcal{N}_\mathcal{A}(\mathcal{G})$ never depends on the metrical properties of the space group $\mathcal{G}$.

If for all space (plane) groups of a certain type the Euclidean normalizers also belong to one type, then for each such space (plane) group the Euclidean and the affine normalizer are identical, irrespective of any metrical specialization, *i.e.* $\mathcal{N}_\mathcal{E}(\mathcal{G}) = \mathcal{N}_\mathcal{A}(\mathcal{G})$ holds. Then, the affine normalizers are pure groups of motions and do not contain any further affine mappings. This is true for all cubic, hexagonal, trigonal and tetragonal space groups (for all hexagonal and square plane groups) and, in addition, for the space groups of 21 further orthorhombic types (plane groups of 4 further rectangular types) [examples: $\mathcal{N}_\mathcal{A}(Pcca) = Pmmm$, $\mathcal{N}_\mathcal{A}(Pnc2) = P^1mmm$].

[2] In previous editions, the symbols Z^1, Z^2 and Z^3 (z^1, z^2) were used.

(*continued on page* 838)

Table 3.5.2.3
Euclidean and chirality-preserving Euclidean normalizers of the monoclinic space groups

For the restrictions of the cell metric see text and Figs. 3.5.2.1 to 3.5.2.4. The symbols in parentheses following a space-group symbol refer to the location of the origin ('origin choice' in Chapter 2.3).

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
3	$P121$	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 121$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/		$(4\cdot\infty)\cdot 1$
		$a>c,\ \beta=90°$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x}, y, z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$(4\cdot\infty)\cdot 2$
		$2\cos\beta=-c/a,\ 90°<\beta<120°$	$B^1 mmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$x, y, x-z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $B^1 222$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$x, \bar{y}, x-z$	$(4\cdot\infty)\cdot 2$
		$a=c,\ 90°<\beta<120°$	$B^1 mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	z, y, x	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $B^1 222$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$z, \bar{y}, x$	$(4\cdot\infty)\cdot 2$
		$a=c,\ \beta=90°$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x}, y, z;\ z, y, x$	$(4\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$\bar{x}, \bar{y}, z;\ z, \bar{y}, x$	$(4\cdot\infty)\cdot 4$
		$a=c,\ \beta=120°$	$P^1 6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$z, y, x;\ \bar{x}+z, y, z$	$(4\cdot\infty)\cdot 2\cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 622$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$z, \bar{y}, x;\ \bar{x}+z, \bar{y}, z$	$(4\cdot\infty)\cdot 6$
3	$P112$	General	$P^1 112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 112$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/		$(4\cdot\infty)\cdot 1$
		$a<b,\ \gamma=90°$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$x, \bar{y}, z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$x, \bar{y}, \bar{z}$	$(4\cdot\infty)\cdot 2$
		$2\cos\gamma=-a/b,\ 90°<\gamma<120°$	$C^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x}+y, y, z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $C^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$\bar{x}+y, y, \bar{z}$	$(4\cdot\infty)\cdot 2$
		$a=b,\ 90°<\gamma<120°$	$C^1 mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $C^1 222$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z}$	$(4\cdot\infty)\cdot 2$
		$a=b,\ \gamma=90°$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x}, y, z;\ y, x, z$	$(4\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$\bar{x}, y, \bar{z};\ y, x, \bar{z}$	$(4\cdot\infty)\cdot 4$
		$a=b,\ \gamma=120°$	$P^1 6/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$y, x, z;\ x, x-y, z$	$(4\cdot\infty)\cdot 2\cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 622$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z};\ x, x-y, \bar{z}$	$(4\cdot\infty)\cdot 6$
4	$P12_11$	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 121$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/		$(4\cdot\infty)\cdot 1$
		$a>c,\ \beta=90°$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x}, y, z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$\bar{x}, \bar{y}, z$	$(4\cdot\infty)\cdot 2$
		$2\cos\beta=-c/a,\ 90°<\beta<120°$	$B^1 mmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$x, y, x-z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $B^1 222$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$x, \bar{y}, x-z$	$(4\cdot\infty)\cdot 2$
		$a=c,\ 90°<\beta<120°$	$B^1 mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	z, y, x	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $B^1 222$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$z, \bar{y}, x$	$(4\cdot\infty)\cdot 2$
		$a=c,\ \beta=90°$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$\bar{x}, y, z;\ z, y, x$	$(4\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$\bar{x}, y, \bar{z};\ z, \bar{y}, x$	$(4\cdot\infty)\cdot 4$
		$a=c,\ \beta=120°$	$P^1 6/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$z, y, x;\ \bar{x}+z, y, z$	$(4\cdot\infty)\cdot 2\cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 622$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2},0,0;\ 0,s,0;\ 0,0,\frac{1}{2}$	/	$z, \bar{y}, x;\ \bar{x}+z, \bar{y}, z$	$(4\cdot\infty)\cdot 6$
4	$P112_1$	General	$P^1 112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 112$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/		$(4\cdot\infty)\cdot 1$
		$a<b,\ \gamma=90°$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x}, y, z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$\bar{x}, y, \bar{z}$	$(4\cdot\infty)\cdot 2$
		$2\cos\gamma=-a/b,\ 90°<\gamma<120°$	$C^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x}+y, y, z$	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $C^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$\bar{x}+y, y, \bar{z}$	$(4\cdot\infty)\cdot 2$
		$a=b,\ 90°<\gamma<120°$	$C^1 mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(4\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $C^1 222$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z}$	$(4\cdot\infty)\cdot 2$
		$a=b,\ \gamma=90°$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$\bar{x}, y, z;\ y, x, z$	$(4\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$\bar{x}, y, \bar{z};\ y, x, \bar{z}$	$(4\cdot\infty)\cdot 4$
		$a=b,\ \gamma=120°$	$P^1 6/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	$y, x, z;\ x, x-y, z$	$(4\cdot\infty)\cdot 2\cdot 6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 622$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	/	$y, x, \bar{z};\ x, x-y, \bar{z}$	$(4\cdot\infty)\cdot 6$

Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
5	$C121$	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 121$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	/		$(2\cdot\infty)\cdot 1$
		$\beta=90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	/	$\bar{x}, y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	$P^1 mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, y, 2x-z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	/	$x, \bar{y}, 2x-z$	$(2\cdot\infty)\cdot 2$
		$2\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	$B^1 mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}+z, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $B^1 222$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	/	$\bar{x}+z, \bar{y}, z$	$(2\cdot\infty)\cdot 2$
		$a=c\sqrt{2},\ \beta=135^\circ$	$P^1 4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, y, 2x-z;\ \bar{x}+z, y, z$	$(2\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}$	$0, s, 0;\ 0, 0, \frac{1}{2}$	/	$x, \bar{y}, 2x-z;\ \bar{x}+z, \bar{y}, z$	$(2\cdot\infty)\cdot 4$
5	$A121$	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 121$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/		$(2\cdot\infty)\cdot 1$
		$\beta=90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$\bar{x}, y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	$\bar{x}+2z, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$\bar{x}+2z, \bar{y}, z$	$(2\cdot\infty)\cdot 2$
		$2\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	$B^1 mmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	$x, y, x-z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $B^1 222$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$x, \bar{y}, x-z$	$(2\cdot\infty)\cdot 2$
		$c=a\sqrt{2},\ \beta=135^\circ$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	$x, y, x-z;\ \bar{x}+2z, y, z$	$(2\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$x, \bar{y}, x-z;\ \bar{x}+2z, \bar{y}, z$	$(2\cdot\infty)\cdot 4$
5	$I121$	General	$P^1 12/m1$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 121$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/		$(2\cdot\infty)\cdot 1$
		$a>c,\ \beta=90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$\bar{x}, \bar{y}, z$	$(2\cdot\infty)\cdot 2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<180^\circ$	$P^1 mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	$x, y, 2x-z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$x, \bar{y}, 2x-z$	$(2\cdot\infty)\cdot 2$
		$a=c,\ 90^\circ<\beta<180^\circ$	$B^1 mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	z, y, x	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $B^1 222$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$z, \bar{y}, x$	$(2\cdot\infty)\cdot 2$
		$a=c,\ \beta=90^\circ$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	$0, 0, 0$	$\bar{x}, y, z;\ z, y, x$	$(2\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, s, 0$	/	$\bar{x}, \bar{y}, z;\ z, \bar{y}, x$	$(2\cdot\infty)\cdot 4$
5	$A112$	General	$P^1 112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 112$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/		$(2\cdot\infty)\cdot 1$
		$\gamma=90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$\bar{x}, y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}+2y, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$\bar{x}+2y, y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$2\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	$C^1 mmm$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	$x, x-y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $C^1 222$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$x, x-y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$b=a\sqrt{2},\ \gamma=135^\circ$	$P^1 4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}+2y, y, z;\ x, x-y, z$	$(2\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$\bar{x}+2y, y, \bar{z};\ x, x-y, \bar{z}$	$(2\cdot\infty)\cdot 4$
5	$B112$	General	$P^1 112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot 2\cdot 1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 112$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	/		$(2\cdot\infty)\cdot 1$
		$\gamma=90^\circ$	$P^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	/	$\bar{x}, y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	$P^1 mmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, 2x-y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 222$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	/	$x, 2x-y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$2\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	$C^1 mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}+y, y, z$	$(2\cdot\infty)\cdot 2\cdot 2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $C^1 222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	/	$\bar{x}+y, y, \bar{z}$	$(2\cdot\infty)\cdot 2$
		$a=b\sqrt{2},\ \gamma=135^\circ$	$P^1 4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, 2x-y, z;\ \bar{x}+y, y, z$	$(2\cdot\infty)\cdot 2\cdot 4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^1 422$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$0, \frac{1}{2}, 0;\ 0, 0, t$	/	$x, 2x-y, \bar{z};\ \bar{x}+y, y, \bar{z}$	$(2\cdot\infty)\cdot 4$

Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
5	$I112$	General	P^1112/m	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty)\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1112	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/		$(2\cdot\infty)\cdot1$
		$a<b,\ \gamma=90^\circ$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty)\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1222	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$\bar{x}, y, \bar{z}$	$(2\cdot\infty)\cdot2$
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<180^\circ$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}+2y, y, z$	$(2\cdot\infty)\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1222	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$\bar{x}+2y, y, \bar{z}$	$(2\cdot\infty)\cdot2$
		$a=b,\ 90^\circ<\gamma<180^\circ$	C^1mmm	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	y, x, z	$(2\cdot\infty)\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: C^1222	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$y, x, \bar{z}$	$(2\cdot\infty)\cdot2$
		$a=b,\ \gamma=90^\circ$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z;\ y, x, z$	$(2\cdot\infty)\cdot2\cdot4$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1422	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, t$	/	$\bar{x}, y, \bar{z};\ y, x, \bar{z}$	$(2\cdot\infty)\cdot4$
6	$P1m1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$a>c,\ \beta=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$2\cos\beta=-c/a,\ 90^\circ<\beta<120^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, y, x-z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=c,\ 90^\circ<\beta<120^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	z, y, x	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=c,\ \beta=90^\circ$	P^24/mmm	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z;\ z, y, x$	$(2\cdot\infty^2)\cdot2\cdot4$
		$a=c,\ \beta=120^\circ$	P^26/mmm	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$z, y, x;\ \bar{x}+z, y, z$	$(2\cdot\infty^2)\cdot2\cdot6$
6	$P11m$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$a<b,\ \gamma=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$2\cos\gamma=-a/b,\ 90^\circ<\gamma<120^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}+y, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=b,\ 90^\circ<\gamma<120^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=b,\ \gamma=90^\circ$	P^24/mmm	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z;\ y, x, z$	$(2\cdot\infty^2)\cdot2\cdot4$
		$a=b,\ \gamma=120^\circ$	P^26/mmm	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$y, x, z;\ x, x-y, z$	$(2\cdot\infty^2)\cdot2\cdot6$
7	$P1c1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$\beta=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}+2z, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$2\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, y, x-z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$c=a\sqrt{2},\ \beta=135^\circ$	P^24/mmm	$\varepsilon\mathbf{a}, -\varepsilon(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, y, x-z;\ \bar{x}+2z, y, z$	$(2\cdot\infty^2)\cdot2\cdot4$
7	$P1n1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$a>c,\ \beta=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<180^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, y, 2x-z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=c,\ 90^\circ<\beta<180^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	z, y, x	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=c,\ \beta=90^\circ$	P^24/mmm	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z;\ z, y, x$	$(2\cdot\infty^2)\cdot2\cdot4$
7	$P1a1$	General	$P^212/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$\beta=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, y, 2x-z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$2\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$\bar{x}+z, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=c\sqrt{2},\ \beta=135^\circ$	P^24/mmm	$-\varepsilon(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{c}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, t$	$0, 0, 0$	$x, y, 2x-z;\ \bar{x}+z, y, z$	$(2\cdot\infty^2)\cdot2\cdot4$
7	$P11a$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$\gamma=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, 2x-y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$2\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}+y, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=b\sqrt{2},\ \gamma=135^\circ$	P^24/mmm	$\varepsilon\mathbf{b}, -\varepsilon(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, 2x-y, z;\ x-y, \bar{y}, z$	$(2\cdot\infty^2)\cdot2\cdot4$
7	$P11n$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$a<b,\ \gamma=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<180^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}+2y, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=b,\ 90^\circ<\gamma<180^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	y, x, z	$(2\cdot\infty^2)\cdot2\cdot2$
		$a=b,\ \gamma=90^\circ$	P^24/mmm	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z;\ y, x, z$	$(2\cdot\infty^2)\cdot2\cdot4$
7	$P11b$	General	P^2112/m	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$		$(2\cdot\infty^2)\cdot2\cdot1$
		$\gamma=90^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	P^2mmm	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}+2y, y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$2\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	P^2mmm	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$x, x-y, z$	$(2\cdot\infty^2)\cdot2\cdot2$
		$b=a\sqrt{2},\ \gamma=135^\circ$	P^24/mmm	$-\varepsilon(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0;\ 0, 0, \frac{1}{2}$	$0, 0, 0$	$\bar{x}+2y, y, z;\ x, x-y, z$	$(2\cdot\infty^2)\cdot2\cdot4$

Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
8	$C1m1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$\beta=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, 2x-z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}+z, y, z$	$\infty^2\cdot 2\cdot 2$
		$a=c\sqrt{2},\ \beta=135^\circ$	$P^2 4/mmm$	$-\varepsilon(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{c}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, 2x-z;\ \bar{x}+z, y, z$	$\infty^2\cdot 2\cdot 4$
8	$A1m1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$\beta=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}+2z, y, z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, x-z$	$\infty^2\cdot 2\cdot 2$
		$c=a\sqrt{2},\ \beta=135^\circ$	$P^2 4/mmm$	$\varepsilon\mathbf{a}, -\varepsilon(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, x-z;\ \bar{x}+2z, y, z$	$\infty^2\cdot 2\cdot 4$
8	$I1m1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$a>c,\ \beta=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<180^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, 2x-z$	$\infty^2\cdot 2\cdot 2$
		$a=c,\ 90^\circ<\beta<180^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	z, y, x	$\infty^2\cdot 2\cdot 2$
		$a=c,\ \beta=90^\circ$	$P^2 4/mmm$	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z;\ z, y, x$	$\infty^2\cdot 2\cdot 4$
8	$A11m$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$\gamma=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+2y, y, z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$x, x-y, z$	$\infty^2\cdot 2\cdot 2$
		$b=a\sqrt{2},\ \gamma=135^\circ$	$P^2 4/mmm$	$-\varepsilon(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+2y, y, z;\ x, x-y, z$	$\infty^2\cdot 2\cdot 4$
8	$B11m$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$\gamma=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$x, 2x-y, z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+y, y, z$	$\infty^2\cdot 2\cdot 2$
		$a=b\sqrt{2},\ \gamma=135^\circ$	$P^2 4/mmm$	$\varepsilon\mathbf{b}, -\varepsilon(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$x, 2x-y, z;\ \bar{x}+y, y, z$	$\infty^2\cdot 2\cdot 4$
8	$I11m$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$a<b,\ \gamma=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<180^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+2y, y, z$	$\infty^2\cdot 2\cdot 2$
		$a=b,\ 90^\circ<\gamma<180^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}-\mathbf{b}), \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	y, x, z	$\infty^2\cdot 2\cdot 2$
		$a=b,\ \gamma=90^\circ$	$P^2 4/mmm$	$\varepsilon\mathbf{a}, \varepsilon\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z;\ y, x, z$	$\infty^2\cdot 2\cdot 4$
9	$C1c1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$\beta=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, 2x-z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	$P^2 bmb$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}+z, y+\frac{1}{4}, z$	$\infty^2\cdot 2\cdot 2$
		$a=c\sqrt{2},\ \beta=135^\circ$	$P^2 4_2/mmc$	$-\varepsilon(\mathbf{a}+\mathbf{c}), \varepsilon\mathbf{c}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, 2x-z;$ $\bar{x}+z, y+\frac{1}{4}, z$	$\infty^2\cdot 2\cdot 4$
9	$A1n1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$\beta=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta=-a/c,\ 90^\circ<\beta<135^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2(\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}+2z, y, z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\beta=-c/a,\ 90^\circ<\beta<135^\circ$	$P^2 bmb$	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y+\frac{1}{4}, x-z$	$\infty^2\cdot 2\cdot 2$
		$c=a\sqrt{2},\ \beta=135^\circ$	$P^2 4_2/mmc$	$\varepsilon\mathbf{a}, -\varepsilon(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y+\frac{1}{4}, x-z;$ $\bar{x}+2z, y, z$	$\infty^2\cdot 2\cdot 4$
9	$I1a1$	General	$P^2 12/m1$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$a>c,\ \beta=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\beta=-c/a,\ 90^\circ<\beta<180^\circ$	$P^2 mmm$	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2\mathbf{c}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$x, y, 2x-z$	$\infty^2\cdot 2\cdot 2$
		$a=c,\ 90^\circ<\beta<180^\circ$	$P^2 bmb$	$\varepsilon_1(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \varepsilon_2(-\mathbf{a}+\mathbf{c})$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$z, y+\frac{1}{4}, x$	$\infty^2\cdot 2\cdot 2$
		$a=c,\ \beta=90^\circ$	$P^2 4_2/mmc$	$\varepsilon\mathbf{c}, \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{b}$	$r, 0, 0;\ 0, 0, t$	0, 0, 0	$\bar{x}, y, z;\ z, y+\frac{1}{4}, x$	$\infty^2\cdot 2\cdot 4$
9	$A11a$	General	$P^2 112/m$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0		$\infty^2\cdot 2\cdot 1$
		$\gamma=90^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot 2\cdot 2$
		$\cos\gamma=-a/b,\ 90^\circ<\gamma<135^\circ$	$P^2 mmm$	$\varepsilon_1\mathbf{a}, \varepsilon_2(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+2y, y, z$	$\infty^2\cdot 2\cdot 2$
		$2\cos\gamma=-b/a,\ 90^\circ<\gamma<135^\circ$	$P^2 ccm$	$\varepsilon_1(\mathbf{a}+\frac{1}{2}\mathbf{b}), \varepsilon_2\mathbf{b}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$x, x-y, z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 2$
		$b=a\sqrt{2},\ \gamma=135^\circ$	$P^2 4_2/mmc$	$-\varepsilon(\mathbf{a}+\mathbf{b}), \varepsilon\mathbf{a}, \frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+2y, y, z;$ $x, x-y, z+\frac{1}{4}$	$\infty^2\cdot 2\cdot 4$

Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
9	$B11n$	General	P^2112/m	$\varepsilon_1\mathbf{a}$, $\varepsilon_2\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0		$\infty^2\cdot2\cdot1$
		$\gamma=90°$	P^2mmm	$\varepsilon_1\mathbf{a}$, $\varepsilon_2\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot2\cdot2$
		$\cos\gamma=-b/a$, $90°<\gamma<135°$	P^2mmm	$\varepsilon_1(\mathbf{a}+\mathbf{b})$, $\varepsilon_2\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$x, 2x-y, z$	$\infty^2\cdot2\cdot2$
		$2\cos\gamma=-a/b$, $90°<\gamma<135°$	P^2ccm	$\varepsilon_1\mathbf{a}$, $\varepsilon_2(\frac{1}{2}\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+y, y, z+\frac{1}{4}$	$\infty^2\cdot2\cdot2$
		$a=b\sqrt{2}$, $\gamma=135°$	P^24_2/mmc	$\varepsilon\mathbf{b}$, $-\varepsilon(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$x, 2x-y, z$; $\bar{x}+y, y, z+\frac{1}{4}$	$\infty^2\cdot2\cdot4$
9	$I11b$	General	P^2112/m	$\varepsilon_1\mathbf{a}$, $\varepsilon_2\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0		$\infty^2\cdot2\cdot1$
		$a<b$, $\gamma=90°$	P^2mmm	$\varepsilon_1\mathbf{a}$, $\varepsilon_2\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z$	$\infty^2\cdot2\cdot2$
		$\cos\gamma=-a/b$, $90°<\gamma<180°$	P^2mmm	$\varepsilon_1\mathbf{a}$, $\varepsilon_2(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}+2y, y, z$	$\infty^2\cdot2\cdot2$
		$a=b$, $90°<\gamma<180°$	P^2ccm	$\varepsilon_1(\mathbf{a}-\mathbf{b})$, $\varepsilon_2(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$y, x, z+\frac{1}{4}$	$\infty^2\cdot2\cdot2$
		$a=b$, $\gamma=90°$	P^24_2/mmc	$\varepsilon\mathbf{a}$, $\varepsilon\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$r, 0, 0;\ 0, s, 0$	0, 0, 0	$\bar{x}, y, z;\ y, x, z+\frac{1}{4}$	$\infty^2\cdot2\cdot4$
10	$P12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			$8\cdot1\cdot1$
		$a>c$, $\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8\cdot1\cdot2$
		$2\cos\beta=-c/a$, $90°<\beta<120°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, x-z$	$8\cdot1\cdot2$
		$a=c$, $90°<\beta<120°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		z, y, x	$8\cdot1\cdot2$
		$a=c$, $\beta=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z;\ z, y, x$	$8\cdot1\cdot4$
		$a=c$, $\beta=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$z, y, x;\ \bar{x}+z, y, z$	$8\cdot1\cdot6$
10	$P112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			$8\cdot1\cdot1$
		$a<b$, $\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8\cdot1\cdot2$
		$2\cos\gamma=-a/b$, $90°<\gamma<120°$	$Cmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{a}+\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+y, y, z$	$8\cdot1\cdot2$
		$a=b$, $90°<\gamma<120°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$8\cdot1\cdot2$
		$a=b$, $\gamma=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z;\ y, x, z$	$8\cdot1\cdot4$
		$a=b$, $\gamma=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$y, x, z;\ x, x-y, z$	$8\cdot1\cdot6$
11	$P12_1/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			$8\cdot1\cdot1$
		$a>c$, $\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8\cdot1\cdot2$
		$2\cos\beta=-c/a$, $90°<\beta<120°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, x-z$	$8\cdot1\cdot2$
		$a=c$, $90°<\beta<120°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		z, y, x	$8\cdot1\cdot2$
		$a=c$, $\beta=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z;\ z, y, x$	$8\cdot1\cdot4$
		$a=c$, $\beta=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$z, y, x;\ \bar{x}+z, y, z$	$8\cdot1\cdot6$
11	$P112_1/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			$8\cdot1\cdot1$
		$a<b$, $\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$8\cdot1\cdot2$
		$2\cos\gamma=-a/b$, $90°<\gamma<120°$	$Cmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{a}+\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+y, y, z$	$8\cdot1\cdot2$
		$a=b$, $90°<\gamma<120°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	$8\cdot1\cdot2$
		$a=b$, $\gamma=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z;\ y, x, z$	$8\cdot1\cdot4$
		$a=b$, $\gamma=120°$	$P6/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$y, x, z;\ x, x-y, z$	$8\cdot1\cdot6$
12	$C12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$			$4\cdot1\cdot1$
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	$4\cdot1\cdot2$
		$\cos\beta=-c/a$, $90°<\beta<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		$x, y, 2x-z$	$4\cdot1\cdot2$
		$2\cos\beta=-a/c$, $90°<\beta<135°$	$Bmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+z, y, z$	$4\cdot1\cdot2$
		$a=c\sqrt{2}$, $\beta=135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, 0, \frac{1}{2}$		$x, y, 2x-z;\ \bar{x}+z, y, z$	$4\cdot1\cdot4$
12	$A12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			$4\cdot1\cdot1$
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	$4\cdot1\cdot2$
		$\cos\beta=-a/c$, $90°<\beta<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}(\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+2z, y, z$	$4\cdot1\cdot2$
		$2\cos\beta=-c/a$, $90°<\beta<135°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, y, x-z$	$4\cdot1\cdot2$
		$c=a\sqrt{2}$, $\beta=135°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $-\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, y, x-z;\ \bar{x}+2z, y, z$	$4\cdot1\cdot4$
12	$I12/m1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			$4\cdot1\cdot1$
		$a>c$, $\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	$4\cdot1\cdot2$
		$\cos\beta=-c/a$, $90°<\beta<180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, y, 2x-z$	$4\cdot1\cdot2$
		$a=c$, $90°<\beta<180°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		z, y, x	$4\cdot1\cdot2$
		$a=c$, $\beta=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}$, $\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z;\ z, y, x$	$4\cdot1\cdot4$

Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
12	$A112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			4·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	4·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+2y, y, z$	4·1·2
		$2\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Cmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, x-y, z$	4·1·2
		$b=a\sqrt{2},\ \gamma=135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+2y, y, z;\ x, x-y, z$	4·1·4
12	$B112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			4·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	4·1·2
		$\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z$	4·1·2
		$2\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+y, y, z$	4·1·2
		$a=b\sqrt{2},\ \gamma=135°$	$P4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z;\ \bar{x}+y, y, z$	4·1·4
12	$I112/m$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			4·1·1
		$a<b,\ \gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	4·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+2y, y, z$	4·1·2
		$a=b,\ 90°<\gamma<180°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		y, x, z	4·1·2
		$a=b,\ \gamma=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z;\ y, x, z$	4·1·4
13	$P12/c1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			8·1·1
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\beta=-a/c,\ 90°<\beta<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c}),$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+2z, y, z$	8·1·2
		$2\cos\beta=-c/a,\ 90°<\beta<135°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, x-z$	8·1·2
		$c=a\sqrt{2},\ \beta=135°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, x-z;\ \bar{x}+2z, y, z$	8·1·4
13	$P12/n1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			8·1·1
		$a>c,\ \beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\beta=-c/a,\ 90°<\beta<180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, 2x-z$	8·1·2
		$a=c,\ 90°<\beta<180°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		z, y, x	8·1·2
		$a=c,\ \beta=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z;\ z, y, x$	8·1·4
13	$P12/a1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			8·1·1
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\beta=-c/a,\ 90°<\beta<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, 2x-z$	8·1·2
		$2\cos\beta=-a/c,\ 90°<\beta<135°$	$Bmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+z, y, z$	8·1·2
		$a=c\sqrt{2},\ \beta=135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, 2x-z;\ \bar{x}+z, y, z$	8·1·4
13	$P112/a$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			8·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, 2x-y, z$	8·1·2
		$2\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+y, y, z$	8·1·2
		$a=b\sqrt{2},\ \gamma=135°$	$P4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, 2x-y, z;\ \bar{x}+y, y, z$	8·1·4
13	$P112/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			8·1·1
		$a<b,\ \gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+2y, y, z$	8·1·2
		$a=b,\ 90°<\gamma<180°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		y, x, z	8·1·2
		$a=b,\ \gamma=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z;\ y, x, z$	8·1·4
13	$P112/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			8·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+2y, y, z$	8·1·2
		$2\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Cmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, x-y, z$	8·1·2
		$b=a\sqrt{2},\ \gamma=135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+2y, y, z;\ x, x-y, z$	8·1·4
14	$P12_1/c1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$			8·1·1
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\beta=-a/c,\ 90°<\beta<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c}),$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$\bar{x}+2z, y, z$	8·1·2
		$2\cos\beta=-c/a,\ 90°<\beta<135°$	$Bmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, x-z$	8·1·2
		$c=a\sqrt{2},\ \beta=135°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0;\ 0, 0, \frac{1}{2}$		$x, y, x-z;\ \bar{x}+2z, y, z$	8·1·4

Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
14	$P12_1/n1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			8·1·1
		$a>c,\ \beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\beta=-c/a,\ 90°<\beta<180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$x, y, 2x-z$	8·1·2
		$a=c,\ 90°<\beta<180°$	$Bmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		z, y, x	8·1·2
		$a=c,\ \beta=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z;\ z, y, x$	8·1·4
14	$P12_1/a1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			8·1·1
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\beta=-c/a,\ 90°<\beta<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$x, y, 2x-z$	8·1·2
		$2\cos\beta=-a/c,\ 90°<\beta<135°$	$Bmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}+z, y, z$	8·1·2
		$a=c\sqrt{2},\ \beta=135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$x, y, 2x-z;\ \bar{x}+z, y, z$	8·1·4
14	$P112_1/a$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			8·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$x, 2x-y, z$	8·1·2
		$2\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Cmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}+y, y, z$	8·1·2
		$a=b\sqrt{2},\ \gamma=135°$	$P4/mmm$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$x, 2x-y, z;\ \bar{x}+y, y, z$	8·1·4
14	$P112_1/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			8·1·1
		$a<b,\ \gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}+2y, y, z$	8·1·2
		$a=b,\ 90°<\gamma<180°$	$Cmmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	8·1·2
		$a=b,\ \gamma=90°$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z;\ y, x, z$	8·1·4
14	$P112_1/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			8·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z$	8·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}+2y, y, z$	8·1·2
		$2\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Cmmm$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$x, x-y, z$	8·1·2
		$b=a\sqrt{2},\ \gamma=135°$	$P4/mmm$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$\bar{x}+2y, y, z;\ x, x-y, z$	8·1·4
15	$C12/c1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			4·1·1
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		$\bar{x}, y, z$	4·1·2
		$\cos\beta=-c/a,\ 90°<\beta<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		$x, y, 2x-z$	4·1·2
		$2\cos\beta=-a/c,\ 90°<\beta<135°$	$Bbmb$ $(n\,2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a}+\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		$\bar{x}+z+\frac{1}{4}, y+\frac{1}{4}, z$	4·1·2
		$a=c\sqrt{2},\ \beta=135°$	$P4_2/mmc$ $(2/m\,2/m\,n)$	$-\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		$x, y, 2x-z;\ \bar{x}+z+\frac{1}{4}, y+\frac{1}{4}, z$	4·1·4
15	$A12/n1$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$			4·1·1
		$\beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}, y, z$	4·1·2
		$\cos\beta=-a/c,\ 90°<\beta<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}(\mathbf{a}+\mathbf{c}),$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}+2z, y, z$	4·1·2
		$2\cos\beta=-c/a,\ 90°<\beta<135°$	$Bbmb$ $(n\,2/m\,n)$	$\mathbf{a}+\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$x, y+\frac{1}{4}, x-z+\frac{1}{4}$	4·1·2
		$c=a\sqrt{2},\ \beta=135°$	$P4_2/mmc$ $(2/m\,2/m\,n)$	$\frac{1}{2}\mathbf{a}, -\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}+2z, y, z;\ x, y+\frac{1}{4}, x-z+\frac{1}{4}$	4·1·4
15	$I12/a1$	General	$P12/m1$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$			4·1·1
		$a>c,\ \beta=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}, y, z$	4·1·2
		$\cos\beta=-c/a,\ 90°<\beta<180°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$x, y, 2x-z$	4·1·2
		$a=c,\ 90°<\beta<180°$	$Bbmb$ $(n\,2/m\,n)$	$\frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}\mathbf{b}, \frac{1}{2}(-\mathbf{a}+\mathbf{c})$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$z+\frac{1}{4}, y+\frac{1}{4}, x+\frac{1}{4}$	4·1·2
		$a=c,\ \beta=90°$	$P4_2/mmc$ $(2/m2/m\,n)$	$\frac{1}{2}\mathbf{c}, \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}, y, z;\ z+\frac{1}{4}, y+\frac{1}{4}, x+\frac{1}{4}$	4·1·4
15	$A112/a$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$			4·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}, y, z$	4·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}+2y, y, z$	4·1·2
		$2\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Cccm$ $(n\,n2/m)$	$\mathbf{a}+\frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$x, x-y+\frac{1}{4}, z+\frac{1}{4}$	4·1·2
		$b=a\sqrt{2},\ \gamma=135°$	$P4_2/mmc$ $(2/m2/m\,n)$	$-\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$\bar{x}+2y, y, z;$ $x, x-y+\frac{1}{4}, z+\frac{1}{4}$	4·1·4

Table 3.5.2.3 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
15	$B112/n$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			4·1·1
		$\gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, \bar{y}, z$	4·1·2
		$\cos\gamma=-b/a,\ 90°<\gamma<135°$	$Pmmm$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z$	4·1·2
		$2\cos\gamma=-a/b,\ 90°<\gamma<135°$	$Cccm$ $(n\,n2/m)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{a}+\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	4·1·2
		$a=b\sqrt{2},\ \gamma=135°$	$P4_2/mmc$ $(2/m2/m\,n)$	$\frac{1}{2}\mathbf{b}, -\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$x, 2x-y, z;$ $\bar{x}+y+\frac{1}{4}, y, z+\frac{1}{4}$	4·1·4
15	$I112/b$	General	$P112/m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$			4·1·1
		$a<b,\ \gamma=90°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z$	4·1·2
		$\cos\gamma=-a/b,\ 90°<\gamma<180°$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}+2y, y, z$	4·1·2
		$a=b,\ 90°<\gamma<180°$	$Cccm$ $(n\,n2/m)$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	4·1·2
		$a=b,\ \gamma=90°$	$P4_2/mmc$ $(2/m2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2}, 0, 0;\ 0, \frac{1}{2}, 0$		$\bar{x}, y, z;\ y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	4·1·4

For each of the other 38 types of orthorhombic space group (3 types of rectangular plane groups), the type of the affine normalizer corresponds to the type of the highest-symmetry Euclidean normalizers belonging to that space (plane)-group type. Therefore, it may also be symbolized by (possibly modified) Hermann–Mauguin symbols [examples: $\mathcal{N}_\mathcal{A}(Pbca) = Pm\bar{3}$, $\mathcal{N}_\mathcal{A}(Pccn) = P4/mmm$, $\mathcal{N}_\mathcal{A}(Pcc2) = P^{1}4/mmm$].

As the affine normalizer of a monoclinic or triclinic space group (oblique plane group) is not isomorphic to any group of motions, it cannot be characterized by a modified Hermann–Mauguin symbol. It may be described, however, by one or two matrix–column pairs together with the appropriate restrictions on the coefficients. Similar information has been given by Billiet *et al.* (1982) for the standard description of each group. The problem has been discussed in more detail by Gubler (1982*a*,*b*).

In Table 3.5.2.6, the affine normalizers of all triclinic and monoclinic space groups are given. The first two columns correspond to those of Tables 3.5.2.3, 3.5.2.4 or 3.5.2.5. The affine normalizers are completely described in column 3 of Table 3.5.2.6 by one or two general matrix–column pairs. All unimodular matrices and columns used in Table 3.5.2.6 are listed explicitly in Table 3.5.2.7. The matrix–column representation of an affine normalizer consists of all combinations of matrices and columns that originate from the specified pair(s) and from the restrictions on the coefficients. This set of matrix–column pairs has of course to include the symmetry operations of $\mathcal{G}$ as well as of $\mathcal{N}_\mathcal{E}(\mathcal{G})$.

The relatively complicated group structure of these affine normalizers has to do with the fact that for the corresponding space groups the permissible basis transformations are more complicated than for space groups of higher crystal systems.

In contrast to orthorhombic space groups, the metric of a triclinic or monoclinic space group cannot be specialized in such a way that all elements of the affine normalizer simultaneously become isometries.

The affine normalizers of the oblique plane groups $p1$ and $p2$ can be described analogously. The corresponding unimodular matrix

$$\begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix}$$

has to be combined with the column

$$\begin{pmatrix} r \\ s \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \end{pmatrix}$$

for the representation of $\mathcal{N}_\mathcal{A}(p1)$ and $\mathcal{N}_\mathcal{A}(p2)$, respectively. n stands for an integer number, r and s stand for real numbers.

3.5.3. Examples of the use of normalizers

By E. Koch and W. Fischer

3.5.3.1. Introduction

The Euclidean and the affine normalizer of a space group form the appropriate tool to define equivalence relationships on sets of objects that are not symmetry-equivalent in this space group but 'play the same role' with respect to this group. Two such objects referring to the same space group will be called Euclidean- or affine-equivalent if there exists a Euclidean or affine mapping that maps the two objects onto one another and, in addition, maps the space group onto itself.

3.5.3.2. Equivalent point configurations, equivalent Wyckoff positions and equivalent descriptions of crystal structures

In the crystal structure of copper, all atoms are symmetry-equivalent with respect to space group $Fm\bar{3}m$. The pattern of Cu atoms may be described equally well by Wyckoff position $4a$ 0, 0, 0 or $4b$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. The Euclidean normalizer of $Fm\bar{3}m$ gives the relation between the two descriptions.

Two *point configurations* (crystallographic orbits)[3] of a space group $\mathcal{G}$ are called *Euclidean-* or *$\mathcal{N}_\mathcal{E}$-equivalent* (*affine-* or *$\mathcal{N}_\mathcal{A}$-equivalent*) if they are mapped onto each other by the Euclidean (affine) normalizer of $\mathcal{G}$.

Affine-equivalent point configurations play the same role with respect to the space-group symmetry, *i.e.* their points are embedded in the pattern of symmetry elements in the same way. Euclidean-equivalent point configurations are congruent and may be interchanged when passing from one description of a crystal structure to another.

[3] For the use of the terms 'point configuration' and 'crystallographic orbit' and a comparison of them, see Koch & Fischer (1985) and Sections 3.4.1 and 3.4.2.

Table 3.5.2.4
Euclidean and chirality-preserving Euclidean normalizers of the orthorhombic space groups

The symbols in parentheses following a space-group symbol refer to the location of the origin ('origin choice' in Chapter 2.3).

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
16	$P222$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0		$8\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$8\cdot1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0	y, x, z	$8\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/	$y, x, \bar{z}$	$8\cdot2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0	$z, x, y;\ y, x, z$	$8\cdot2\cdot6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/	$z, x, y;\ y, x, \bar{z}$	$8\cdot6$
17	$P222_1$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0		$8\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$8\cdot1$
		$a = b$	$P4_2/mmc$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0	$y, x, z+\frac{1}{4}$	$8\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/	$y, x, \bar{z}+\frac{1}{4}$	$8\cdot2$
18	$P2_12_12$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0		$8\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$8\cdot1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0	y, x, z	$8\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/	$y, x, \bar{z}$	$8\cdot2$
19	$P2_12_12_1$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0		$8\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$8\cdot1$
		$a = b \neq c$	$P4_2/mmc$ $(2/m\,2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$8\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$ (222_1)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/	$\bar{y}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{z}+\frac{1}{4}$	$8\cdot2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	0, 0, 0	$z, x, y;\ y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$8\cdot2\cdot6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_232$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/	$z, x, y;\ \bar{y}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{z}+\frac{1}{4}$	$8\cdot6$
20	$C222_1$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	0, 0, 0		$4\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	/		$4\cdot1$
		$a = b$	$P4_2/mmc$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	0, 0, 0	$y, x, z+\frac{1}{4}$	$4\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	/	$y, x, \bar{z}+\frac{1}{4}$	$4\cdot2$
21	$C222$	$a \neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	0, 0, 0		$4\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	/		$4\cdot1$
		$a = b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	0, 0, 0	y, x, z	$4\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$	/	$y, x, \bar{z}$	$4\cdot2$
22	$F222$	$a \neq b \neq c \neq a$	$Immm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	0, 0, 0		$4\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	/		$4\cdot1$
		$a = b \neq c$	$I4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	0, 0, 0	y, x, z	$4\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	/	$y, x, \bar{z}$	$4\cdot2$
		$a = b = c$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	0, 0, 0	$z, x, y;\ y, x, z$	$4\cdot2\cdot6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	/	$z, x, y;\ y, x, \bar{z}$	$4\cdot6$
23	$I222$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	0, 0, 0		$4\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	/		$4\cdot1$
		$a = b \neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	0, 0, 0	y, x, z	$4\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	/	$y, x, \bar{z}$	$4\cdot2$
		$a = b = c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	0, 0, 0	$z, x, y;\ y, x, z$	$4\cdot2\cdot6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	/	$z, x, y;\ y, x, \bar{z}$	$4\cdot6$
24	$I2_12_12_1$	$a \neq b \neq c \neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	0, 0, 0		$4\cdot2\cdot1$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P222$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	/		$4\cdot1$
		$a = b \neq c$	$P4_2/mmc$ $(2/m\,2/m\,n)$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	0, 0, 0	$y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$4\cdot2\cdot2$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$ (222_1)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	/	$\bar{y}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{z}+\frac{1}{4}$	$4\cdot2$
		$a = b = c$	$Pm\bar{3}n$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	0, 0, 0	$z, x, y;\ y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$	$4\cdot2\cdot6$
			$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_232$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$	/	$z, x, y;\ \bar{y}+\frac{1}{4}, \bar{x}+\frac{1}{4}, \bar{z}+\frac{1}{4}$	$4\cdot6$
25	$Pmm2$	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot2\cdot1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(4\cdot\infty)\cdot2\cdot2$
26	$Pmc2_1$		P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot2\cdot1$
27	$Pcc2$	$a \neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot2\cdot1$
		$a = b$	P^14/mmm	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(4\cdot\infty)\cdot2\cdot2$

Table 3.5.2.4 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
28	*Pma*2		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
29	*Pca*2_1		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
30	*Pnc*2		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
31	*Pmn*2_1		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
32	*Pba*2	$a\neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
		$a=b$	P^14/mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(4\cdot\infty)\cdot 2\cdot 2$
33	*Pna*2_1		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
34	*Pnn*2	$a\neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0		$(4\cdot\infty)\cdot 2\cdot 1$
		$a=b$	P^14/mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,t$	0, 0, 0	y, x, z	$(4\cdot\infty)\cdot 2\cdot 2$
35	*Cmm*2	$a\neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
		$a=b$	P^14/mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
36	*Cmc*2_1		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
37	*Ccc*2	$a\neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
		$a=b$	P^14/mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
38	*Amm*2		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
39	*Aem*2		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
40	*Ama*2		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
41	*Aea*2		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
42	*Fmm*2	$a\neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	0, 0, 0		$\infty\cdot 2\cdot 1$
		$a=b$	P^14/mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	0, 0, 0	y, x, z	$\infty\cdot 2\cdot 2$
43	*Fdd*2	$a\neq b$	P^1ban (222)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$\frac{1}{8},\frac{1}{8},0$		$\infty\cdot 2\cdot 1$
		$a=b$	P^14/nbm ($\bar{4}2m$)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$\frac{1}{8},\frac{1}{8},0$	y, x, z	$\infty\cdot 2\cdot 2$
44	*Imm*2	$a\neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
		$a=b$	P^14/mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
45	*Iba*2	$a\neq b$	P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
		$a=b$	P^14/mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0	y, x, z	$(2\cdot\infty)\cdot 2\cdot 2$
46	*Ima*2		P^1mmm	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,t$	0, 0, 0		$(2\cdot\infty)\cdot 2\cdot 1$
47	*Pmmm*	$a\neq b\neq c\neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a=b\neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
		$a=b=c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$z, x, y;\ y, x, z$	$8\cdot 1\cdot 6$
48	*Pnnn* (both	$a\neq b\neq c\neq a$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
	origins)	$a=b\neq c$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
		$a=b=c$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		$z, x, y;\ y, x, z$	$8\cdot 1\cdot 6$
49	*Pccm*	$a\neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a=b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
50	*Pban* (both	$a\neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
	origins)	$a=b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
51	*Pmma*		$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
52	*Pnna*		$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
53	*Pmna*		$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
54	*Pcca*		$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
55	*Pbam*	$a\neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a=b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
56	*Pccn*	$a\neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a=b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
57	*Pbcm*		$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
58	*Pnnm*	$a\neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
		$a=b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
59	*Pmmn* (both	$a\neq b$	$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$
	origins)	$a=b$	$P4/mmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y, x, z	$8\cdot 1\cdot 2$
60	*Pbcn*		$Pmmm$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot 1\cdot 1$

Table 3.5.2.4 (continued)

Space group $\mathcal{G}$			Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Cell metric	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
61	*Pbca*	$a \neq b$ or $b \neq c$ or $a \neq c$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot1\cdot1$
		$a=b=c$	*Pm*$\bar{3}$	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$		z,x,y	$8\cdot1\cdot3$
62	*Pnma*		*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$8\cdot1\cdot1$
63	*Cmcm*		*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
64	*Cmce*		*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
65	*Cmmm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
		$a=b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot1\cdot2$
66	*Cccm*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
		$a=b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot1\cdot2$
67	*Cmme*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
		$a=b$	*P*4/*mmm* (*mmm*)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		$y+\frac{1}{4},x-\frac{1}{4},z$	$4\cdot1\cdot2$
68	*Ccce* (222)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
		$a=b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot1\cdot2$
68	*Ccce* ($\bar{1}$)	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
		$a=b$	*P*4/*mmm* (*mmm*)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,0,\frac{1}{2}$		$y+\frac{1}{4},x-\frac{1}{4},z$	$4\cdot1\cdot2$
69	*Fmmm*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$			$2\cdot1\cdot1$
		$a=b\neq c$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		y,x,z	$2\cdot1\cdot2$
		$a=b=c$	*Pm*$\bar{3}$*m*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$z,x,y;\ y,x,z$	$2\cdot1\cdot6$
70	*Fddd* (222)	$a \neq b \neq c \neq a$	*Pnnn* (222)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$			$2\cdot1\cdot1$
		$a=b\neq c$	*P*4$_2$/*nnm* ($\bar{4}2m$)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$\bar{y},\bar{x},z$	$2\cdot1\cdot2$
		$a=b=c$	*Pn*$\bar{3}$*m* ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$z,x,y;\ y,x,z$	$2\cdot1\cdot6$
70	*Fddd* ($\bar{1}$)	$a \neq b \neq c \neq a$	*Pnnn* ($\bar{1}$)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$			$2\cdot1\cdot1$
		$a=b\neq c$	*P*4$_2$/*nnm* (2/*m* at $0,\frac{1}{2},0$)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		y,x,z	$2\cdot1\cdot2$
		$a=b=c$	*Pn*$\bar{3}$*m* ($\bar{3}m$)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0$		$z,x,y;\ y,x,z$	$2\cdot1\cdot6$
71	*Immm*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$a=b\neq c$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		y,x,z	$4\cdot1\cdot2$
		$a=b=c$	*Pm*$\bar{3}$*m*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$z,x,y;\ y,x,z$	$4\cdot1\cdot6$
72	*Ibam*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$a=b$	*P*4/*mmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		y,x,z	$4\cdot1\cdot2$
73	*Ibca*	$a \neq b \neq c \neq a$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$a=b\neq c$	*P*4$_2$/*mmc* (2/*m*2/*m n*)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	$4\cdot1\cdot2$
		$a=b=c$	*Pm*$\bar{3}$*n*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$z,x,y;\ y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	$4\cdot1\cdot6$
74	*Imma*	$a \neq b$	*Pmmm*	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$			$4\cdot1\cdot1$
		$a=b$	*P*4$_2$/*mmc* (2/*m*2/*m n*)	$\frac{1}{2}\mathbf{a}$, $\frac{1}{2}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,0;\ 0,\frac{1}{2},0$		$y+\frac{1}{4},x-\frac{1}{4},z+\frac{1}{4}$	$4\cdot1\cdot2$

Starting from any given point configuration of a space group $\mathcal{G}$, one may derive all Euclidean-equivalent point configurations and – except for monoclinic and triclinic space groups – all affine-equivalent ones by successive application of the 'additional generators' of the normalizer as given in Tables 3.5.2.3, 3.5.2.4 and 3.5.2.5.

Examples

(1) A point configuration $F\bar{4}3m$ 16*e* x,x,x with $x_1 = 0.10$ may be visualized as a set of parallel tetrahedra arranged in a cubic face-centred lattice. The Euclidean and affine normalizer of $F\bar{4}3m$ is $Im\bar{3}m$ with $a' = \frac{1}{2}a$ (*cf.* Table 3.5.2.5). Since the index k_g of $\mathcal{G}$ in $\mathcal{K}(\mathcal{G})$ is 4, three additional equivalent point configurations exist, which follow from the original one by repeated application of the tabulated translation $t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$: 16*e* x,x,x with $x_2 = 0.35$, $x_3 = 0.60$, $x_4 = 0.85$. $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{K}(\mathcal{G})$ and an additional centre of symmetry is located at 0, 0, 0. Accordingly, the following four equivalent point configurations may be derived from the first four: 16*e* x,x,x with $x_5 = -0.10$, $x_6 = -0.35$, $x_7 = -0.60$, $x_8 = -0.85$. In this case, the index 8 of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$ equals the number of Euclidean-equivalent point configurations.

(2) $F\bar{4}3m$ 4*a* 0, 0, 0 represents a face-centred cubic lattice. The additional translations of $\mathcal{K}(F\bar{4}3m)$ generate three equivalent point configurations: 4*c* $\frac{1}{4},\frac{1}{4},\frac{1}{4}$, 4*b* $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ and 4*d* $\frac{3}{4},\frac{3}{4},\frac{3}{4}$. Inversion through 0, 0, 0 maps 4*a* and 4*b* each onto itself and interchanges 4*c* and 4*d*. Therefore, here the number of equivalent point configurations is four, *i.e.* only half the index of $\mathcal{G}$ in $\mathcal{N}_\mathcal{E}(\mathcal{G})$.

The difference between the two examples is the following: The reference point 0.1, 0.1, 0.1 of the first example does not change its site symmetry .3*m* when passing from $F\bar{4}3m$ to $Im\bar{3}m$. Point 0, 0, 0 of the second example, however, has site symmetry $\bar{4}3m$ in $F\bar{4}3m$, but $m\bar{3}m$ in $Im\bar{3}m$.

(*continued on page* 846)

Table 3.5.2.5
Euclidean and chirality-preserving Euclidean normalizers of the tetragonal, trigonal, hexagonal and cubic space groups
The symbols in parentheses following a space-group symbol refer to the location of the origin ('origin choice' in Chapter 2.3).

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	
75	$P4$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$	y,x,z	$(2\cdot\infty)\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^{1}422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y,x,\bar{z}$	$(2\cdot\infty)\cdot 2$
76	$P4_1$	$P^{1}422$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y,x,\bar{z}$	$(2\cdot\infty)\cdot 2$
77	$P4_2$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$	y,x,z	$(2\cdot\infty)\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^{1}422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y,x,\bar{z}$	$(2\cdot\infty)\cdot 2$
78	$P4_3$	$P^{1}422$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	/	$y,x,\bar{z}$	$(2\cdot\infty)\cdot 2$
79	$I4$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$	y,x,z	$\infty\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^{1}422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot 2$
80	$I4_1$	$P^{1}4/nbm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	$\frac{1}{4},0,0$	$y,x,\bar{z}$	$\infty\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^{1}422$ (222)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot 2$
81	$P\bar{4}$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$	y,x,z	$4\cdot 2\cdot 2$
82	$I\bar{4}$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,\frac{1}{4}$	$0,0,0$	y,x,z	$4\cdot 2\cdot 2$
83	$P4/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot 1\cdot 2$
84	$P4_2/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot 1\cdot 2$
85	$P4/n$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot 1\cdot 2$
85	$P4/n$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot 1\cdot 2$
86	$P4_2/n$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot 1\cdot 2$
86	$P4_2/n$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$		y,x,z	$4\cdot 1\cdot 2$
87	$I4/m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$
88	$I4_1/a$ ($\bar{4}$)	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$y,x,\bar{z}$	$2\cdot 1\cdot 2$
88	$I4_1/a$ ($\bar{1}$)	$P4_2/nnm$ ($2/m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	$2\cdot 1\cdot 2$
89	$P422$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
90	$P42_12$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
91	$P4_122$	$P4_222$ (222 at 4_212) [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
92	$P4_12_12$	$P4_222$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
93	$P4_222$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
94	$P4_22_12$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
95	$P4_322$	$P4_222$ (222 at 4_212) [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
96	$P4_32_12$	$P4_222$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	/		$4\cdot 1$
97	$I422$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P422$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot 1$
98	$I4_122$	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$\frac{1}{4},0,\frac{1}{8}$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_222$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot 1$
99	$P4mm$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
100	$P4bm$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
101	$P4_2cm$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
102	$P4_2nm$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
103	$P4cc$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
104	$P4nc$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
105	$P4_2mc$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
106	$P4_2bc$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,t$	$0,0,0$		$(2\cdot\infty)\cdot 2\cdot 1$
107	$I4mm$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot 2\cdot 1$
108	$I4cm$	$P^{1}4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot 2\cdot 1$
109	$I4_1md$	$P^{1}4/nbm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	$\frac{1}{4},0,0$		$\infty\cdot 2\cdot 1$
110	$I4_1cd$	$P^{1}4/nbm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \varepsilon\mathbf{c}$	$0,0,t$	$\frac{1}{4},0,0$		$\infty\cdot 2\cdot 1$
111	$P\bar{4}2m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
112	$P\bar{4}2c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$
113	$P\bar{4}2_1m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b}),\ \frac{1}{2}(\mathbf{a}+\mathbf{b}),\ \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot 2\cdot 1$

Table 3.5.2.5 (continued)

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
114	$P\bar{4}2_1c$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot2\cdot1$
115	$P\bar{4}m2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot2\cdot1$
116	$P\bar{4}c2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot2\cdot1$
117	$P\bar{4}b2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot2\cdot1$
118	$P\bar{4}n2$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$4\cdot2\cdot1$
119	$I\bar{4}m2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,\frac{1}{4}$	$0,0,0$		$4\cdot2\cdot1$
120	$I\bar{4}c2$	$I4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},0,\frac{1}{4}$	$0,0,0$		$4\cdot2\cdot1$
121	$I\bar{4}2m$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot2\cdot1$
122	$I\bar{4}2d$	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$\frac{1}{4},0,\frac{1}{8}$		$2\cdot2\cdot1$
123	$P4/mmm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
124	$P4/mcc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
125	$P4/nbm$ (422)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
125	$P4/nbm$ (2/m)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
126	$P4/nnc$ (422)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
126	$P4/nnc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
127	$P4/mbm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
128	$P4/mnc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
129	$P4/nmm$ ($\bar{4}m2$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
129	$P4/nmm$ (2/m)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
130	$P4/ncc$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
130	$P4/ncc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
131	$P4_2/mmc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
132	$P4_2/mcm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
133	$P4_2/nbc$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
133	$P4_2/nbc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
134	$P4_2/nnm$ ($\bar{4}2m$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
134	$P4_2/nnm$ (2/m)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
135	$P4_2/mbc$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
136	$P4_2/mnm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
137	$P4_2/nmc$ ($\bar{4}m2$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
137	$P4_2/nmc$ ($\bar{1}$)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
138	$P4_2/ncm$ ($\bar{4}$)	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
138	$P4_2/ncm$ (2/m)	$P4/mmm$ (mmm)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},0;\ 0,0,\frac{1}{2}$			$4\cdot1\cdot1$
139	$I4/mmm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
140	$I4/mcm$	$P4/mmm$	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
141	$I4_1/amd$ ($\bar{4}m2$)	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
141	$I4_1/amd$ (2/m)	$P4_2/nnm$ (2/m)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
142	$I4_1/acd$ ($\bar{4}$)	$P4_2/nnm$ ($\bar{4}2m$)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
142	$I4_1/acd$ ($\bar{1}$)	$P4_2/nnm$ (2/m)	$\frac{1}{2}(\mathbf{a}-\mathbf{b})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b})$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
143	$P3$	$P^1 6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	$0,0,0$	$\bar{x},\bar{y},z;\ y,x,z$	$(3\cdot\infty)\cdot2\cdot4$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1622	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	/	$\bar{x},\bar{y},z;\ y,x,\bar{z}$	$(3\cdot\infty)\cdot4$
144	$P3_1$	P^1622 [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	/	$\bar{x},\bar{y},z;\ y,x,\bar{z}$	$(3\cdot\infty)\cdot4$
145	$P3_2$	P^1622 [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,t$	/	$\bar{x},\bar{y},z;\ y,x,\bar{z}$	$(3\cdot\infty)\cdot4$
146	$R3$ (hexag.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$	$\bar{y},\bar{x},z$	$\infty\cdot2\cdot2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1312	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot2$
146	$R3$ (rhomboh.)	$P^1\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $\varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r,r,r	$0,0,0$	y,x,z	$\infty\cdot2\cdot2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: P^1312	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $\varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r,r,r	/	$\bar{y},\bar{x},\bar{z}$	$\infty\cdot2$
147	$P\bar{3}$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{x},\bar{y},z;\ y,x,z$	$2\cdot1\cdot4$
148	$R\bar{3}$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}$, $-\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{y},\bar{x},z$	$2\cdot1\cdot2$
148	$R\bar{3}$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot1\cdot2$

Table 3.5.2.5 (continued)

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
149	$P312$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0$; $0,0,\frac{1}{2}$	$0,0,0$	$\bar{x},\bar{y},z$	$6\cdot2\cdot2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P622$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0$; $0,0,\frac{1}{2}$	/	$\bar{x},\bar{y},z$	$6\cdot2$
150	$P321$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$	$\bar{x},\bar{y},z$	$2\cdot2\cdot2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P622$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/	$\bar{x},\bar{y},z$	$2\cdot2$
151	$P3_112$	$P6_222$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0$; $0,0,\frac{1}{2}$	/	$\bar{x},\bar{y},z$	$6\cdot2$
152	$P3_121$	$P6_222$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}+\mathbf{b}$, $-\mathbf{a}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/	$\bar{x},\bar{y},z$	$2\cdot2$
153	$P3_212$	$P6_422$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0$; $0,0,\frac{1}{2}$	/	$\bar{x},\bar{y},z$	$6\cdot2$
154	$P3_221$	$P6_422$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}+\mathbf{b}$, $-\mathbf{a}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/	$\bar{x},\bar{y},z$	$2\cdot2$
155	$R32$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}$, $-\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot2\cdot1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $R32$ (hexag.)	$-\mathbf{a}$, $-\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot1$
155	$R32$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$		$2\cdot2\cdot1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $R32$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/		$2\cdot1$
156	$P3m1$	$P^{1}6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0$; $0,0,t$	$0,0,0$	$\bar{x},\bar{y},z$	$(3\cdot\infty)\cdot2\cdot2$
157	$P31m$	$P^{1}6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$	$\bar{x},\bar{y},z$	$\infty\cdot2\cdot2$
158	$P3c1$	$P^{1}6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0$; $0,0,t$	$0,0,0$	$\bar{x},\bar{y},z$	$(3\cdot\infty)\cdot2\cdot2$
159	$P31c$	$P^{1}6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$	$\bar{x},\bar{y},z$	$\infty\cdot2\cdot2$
160	$R3m$ (hexag.)	$P^{1}\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot2\cdot1$
160	$R3m$ (rhomboh.)	$P^{1}\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $\varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r,r,r	$0,0,0$		$\infty\cdot2\cdot1$
161	$R3c$ (hexag.)	$P^{1}\bar{3}1m$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot2\cdot1$
161	$R3c$ (rhomboh.)	$P^{1}\bar{3}1m$	$\frac{2}{3}\mathbf{a}-\frac{1}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $-\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}-\frac{1}{3}\mathbf{c}$, $\varepsilon(\mathbf{a}+\mathbf{b}+\mathbf{c})$	r,r,r	$0,0,0$		$\infty\cdot2\cdot1$
162	$P\bar{3}1m$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{x},\bar{y},z$	$2\cdot1\cdot2$
163	$P\bar{3}1c$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{x},\bar{y},z$	$2\cdot1\cdot2$
164	$P\bar{3}m1$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{x},\bar{y},z$	$2\cdot1\cdot2$
165	$P\bar{3}c1$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		$\bar{x},\bar{y},z$	$2\cdot1\cdot2$
166	$R\bar{3}m$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}$, $-\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
166	$R\bar{3}m$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
167	$R\bar{3}c$ (hexag.)	$R\bar{3}m$ (hexag.)	$-\mathbf{a}$, $-\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot1\cdot1$
167	$R\bar{3}c$ (rhomboh.)	$R\bar{3}m$ (rhomboh.)	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$, $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
168	$P6$	$P^{1}6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$	y,x,z	$\infty\cdot2\cdot2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^{1}622$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot2$
169	$P6_1$	$P^{1}622$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot2$
170	$P6_5$	$P^{1}622$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot2$
171	$P6_2$	$P^{1}622$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot2$
172	$P6_4$	$P^{1}622$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot2$
173	$P6_3$	$P^{1}6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$	y,x,z	$\infty\cdot2\cdot2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P^{1}622$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	/	$y,x,\bar{z}$	$\infty\cdot2$
174	$P\bar{6}$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $-\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0$; $0,0,\frac{1}{2}$	$0,0,0$	y,x,z	$6\cdot2\cdot2$
175	$P6/m$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		y,x,z	$2\cdot1\cdot2$
176	$P6_3/m$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$		y,x,z	$2\cdot1\cdot2$
177	$P622$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot2\cdot1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P622$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot1$
178	$P6_122$	$P6_222$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot1$
179	$P6_522$	$P6_422$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot1$
180	$P6_222$	$P6_422$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot1$
181	$P6_422$	$P6_222$ [$\equiv\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot1$
182	$P6_322$	$P6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot2\cdot1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P622$	$\mathbf{a}$, $\mathbf{b}$, $\frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	/		$2\cdot1$
183	$P6mm$	$P^{1}6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot2\cdot1$
184	$P6cc$	$P^{1}6/mmm$	$\mathbf{a}$, $\mathbf{b}$, $\varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot2\cdot1$

Table 3.5.2.5 (continued)

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
185	$P6_3cm$	$P^{1}6/mmm$	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot 2\cdot 1$
186	$P6_3mc$	$P^{1}6/mmm$	$\mathbf{a}, \mathbf{b}, \varepsilon\mathbf{c}$	$0,0,t$	$0,0,0$		$\infty\cdot 2\cdot 1$
187	$P\bar{6}m2$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$6\cdot 2\cdot 1$
188	$P\bar{6}c2$	$P6/mmm$	$\frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ -\frac{1}{3}\mathbf{a}+\frac{1}{3}\mathbf{b},\ \frac{1}{2}\mathbf{c}$	$\frac{2}{3},\frac{1}{3},0;\ 0,0,\frac{1}{2}$	$0,0,0$		$6\cdot 2\cdot 1$
189	$P\bar{6}2m$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
190	$P\bar{6}2c$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
191	$P6/mmm$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
192	$P6/mcc$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
193	$P6_3/mcm$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
194	$P6_3/mmc$	$P6/mmm$	$\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$	$0,0,\frac{1}{2}$			$2\cdot 1\cdot 1$
195	$P23$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$	y,x,z	$2\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/	$y,x,\bar{z}$	$2\cdot 2$
196	$F23$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$0,0,0$	y,x,z	$4\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	/	$y,x,\bar{z}$	$4\cdot 2$
197	$I23$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0,0,0$	y,x,z	$1\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		/	$y,x,\bar{z}$	$1\cdot 2$
198	$P2_13$	$Ia\bar{3}d$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$	$y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	$2\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I4_132$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/	$\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	$2\cdot 2$
199	$I2_13$	$Ia\bar{3}d$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0,0,0$	$y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	$1\cdot 2\cdot 2$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I4_132$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		/	$\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	$1\cdot 2$
200	$Pm\bar{3}$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$
201	$Pn\bar{3}$ (23)	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$
201	$Pn\bar{3}$ ($\bar{3}$)	$Im\bar{3}m$ ($\bar{3}m$)	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$
202	$Fm\bar{3}$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$
203	$Fd\bar{3}$ (23)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$
203	$Fd\bar{3}$ ($\bar{3}$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		y,x,z	$2\cdot 1\cdot 2$
204	$Im\bar{3}$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$			y,x,z	$1\cdot 1\cdot 2$
205	$Pa\bar{3}$	$Ia\bar{3}$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot 1\cdot 1$
206	$Ia\bar{3}$	$Ia\bar{3}d$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$			$y+\frac{1}{4},x+\frac{1}{4},z+\frac{1}{4}$	$1\cdot 1\cdot 2$
207	$P432$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/		$2\cdot 1$
208	$P4_232$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/		$2\cdot 1$
209	$F432$	$Pm\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P432$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/		$2\cdot 1$
210	$F4_132$	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$		$2\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $P4_232$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/		$2\cdot 1$
211	$I432$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0,0,0$		$1\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I432$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		/		$1\cdot 1$
212	$P4_332$	$I4_132$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/		$2\cdot 1$
213	$P4_132$	$I4_132$ [$\equiv \mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$]	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	/		$2\cdot 1$
214	$I4_132$	$Ia\bar{3}d$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0,0,0$		$1\cdot 2\cdot 1$
		$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$: $I4_132$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		/		$1\cdot 1$
215	$P\bar{4}3m$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
216	$F\bar{4}3m$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$0,0,0$		$4\cdot 2\cdot 1$
217	$I\bar{4}3m$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0,0,0$		$1\cdot 2\cdot 1$
218	$P\bar{4}3n$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,0$		$2\cdot 2\cdot 1$
219	$F\bar{4}3c$	$Im\bar{3}m$	$\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$0,0,0$		$4\cdot 2\cdot 1$
220	$I\bar{4}3d$	$Ia\bar{3}d$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$		$0,0,0$		$1\cdot 2\cdot 1$
221	$Pm\bar{3}m$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot 1\cdot 1$
222	$Pn\bar{3}n$ (432)	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot 1\cdot 1$
222	$Pn\bar{3}n$ ($\bar{3}$)	$Im\bar{3}m$ ($\bar{3}m$)	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot 1\cdot 1$
223	$Pm\bar{3}n$	$Im\bar{3}m$	$\mathbf{a}, \mathbf{b}, \mathbf{c}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot 1\cdot 1$

Table 3.5.2.5 (continued)

Space group $\mathcal{G}$		Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and chirality-preserving normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$		Additional generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ and $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$			
No.	Hermann–Mauguin symbol	Symbol	Basis vectors	Translations	Inversion through a centre at	Further generators	Index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ or $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$
224	$Pn\bar{3}m$ ($\bar{4}3m$)	$Im\bar{3}m$	**a**, **b**, **c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
224	$Pn\bar{3}m$ ($\bar{3}m$)	$Im\bar{3}m$ ($\bar{3}m$)	**a**, **b**, **c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
225	$Fm\bar{3}m$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
226	$Fm\bar{3}c$	$Pm\bar{3}m$	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
227	$Fd\bar{3}m$ ($\bar{4}3m$)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
227	$Fd\bar{3}m$ ($\bar{3}m$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
228	$Fd\bar{3}c$ (23)	$Pn\bar{3}m$ ($\bar{4}3m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
228	$Fd\bar{3}c$ ($\bar{3}$)	$Pn\bar{3}m$ ($\bar{3}m$)	$\frac{1}{2}$**a**, $\frac{1}{2}$**b**, $\frac{1}{2}$**c**	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			$2\cdot1\cdot1$
229	$Im\bar{3}m$	$Im\bar{3}m$	**a**, **b**, **c**				$1\cdot1\cdot1$
230	$Ia\bar{3}d$	$Ia\bar{3}d$	**a**, **b**, **c**				$1\cdot1\cdot1$

The following rule holds without exception: The number of point configurations equivalent to a given one is equal to the quotient i/i_s, with i being the subgroup index of $\mathcal{G}$ in its Euclidean or affine normalizer and i_s the subgroup index between the corresponding two site-symmetry groups of any point in the original point configuration.

When referring to the Euclidean normalizer, i_s may be higher than 1 only if the eigensymmetry of the point configuration under consideration (*i.e.* the group of all motions that maps the point configuration onto itself, *cf.* Sections 1.4.4.4 and 3.4.1.3) is a proper supergroup of $\mathcal{G}$. If $\mathcal{D}$ designates the intersection group of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ with the eigensymmetry group of the point configuration, the number of Euclidean-equivalent point configurations equals the index of $\mathcal{D}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example

The Euclidean and affine normalizer of $P2_13$ is $Ia\bar{3}d$ with index 8. Point configuration $4a\ x,x,x$ with $x_1 = 0$ forms a face-centred cubic lattice with eigensymmetry $Fm\bar{3}m$. The reference point $0,0,0$ has site symmetry .3. in $P2_13$ but .$\bar{3}$. in $Ia\bar{3}d$. The number of equivalent point configurations, therefore, is $i/i_s = 8/2 = 4$. One additional point configuration is generated by the translation $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$: $4a\ x,x,x$ with $x_2 = \frac{1}{2}$, the two others by applying the d-glide reflection $y+\frac{1}{4}, x+\frac{1}{4}, z+\frac{1}{4}$ to the first two point configurations: $4a\ x,x,x$ with $x_3 = \frac{1}{4}$ and $x_4 = \frac{3}{4}$. The intersection group $\mathcal{D}$ of the eigensymmetry $Fm\bar{3}m$ with the normalizer $Ia\bar{3}d$ is $Pa\bar{3}$. Its index 4 in $Ia\bar{3}d$ gives again the number of equivalent point configurations.

The set of equivalent point configurations is always infinite if the normalizer contains continuous translations, but this set may be described by a finite number of subsets due to non-continuous translations.

Example

The Euclidean and affine normalizer of $P6_1$ is $P^{1}622$ (**a**, **b**, ε**c**). With the aid of the 'additional generators' given in Table 3.5.2.5, one can calculate two subsets of point configurations that are equivalent to a given general point configuration $6a\ x,y,z$ with $x = x_0,\ y = y_0,\ z = z_0$: $6a\ x,y,z$ with x_0, y_0, z_0+t and $y_0, x_0, -z_0+t$. If, however, the coordinates for the original point configuration are specialized, *e.g.* to $x = y = x_1,\ z = z_1$ or to $x = y = 0,\ z = z_2$, only one subset exists, namely x_1, x_1, z_1+t or $0,0,z_2+t$, respectively. The reduction of the number of subsets is a consequence of the enhancement of the site symmetry in the normalizer (.2. or 622, respectively), but the index i_s, as introduced above, does not necessarily give the reduction factor for the number of subsets.

It has to be noticed that for most space groups with a Euclidean normalizer containing continuous translations the index i_s is larger than 1 for *all* point configurations, *i.e.* the number of subsets of equivalent point configurations is necessarily reduced. The general Wyckoff position of such a space group does not belong to a characteristic type of Wyckoff sets (*cf.* Sections 1.4.4 and 3.4.1.3) and the eigensymmetry of all corresponding point configurations is enhanced.

Example

The Euclidean and affine normalizer of $P6$ is $P^{1}6/mmm$ (**a**, **b**, ε**c**). As a consequence of the continuous translations, the site symmetry of any point is at least m.. in $P^{1}6/mmm$. With the aid of the 'additional generators', one calculates four subsets of point configurations that are equivalent to a given general point configuration $6d\ x,y,z$ with $x = x_0,\ y = y_0,\ z = z_0$: x_0, y_0, z_0+t; $-x_0, -y_0, -z_0+t$; y_0, x_0, z_0+t; $-y_0, -x_0, -z_0+t$. The first two and the second two subsets coincide, however.

According to the above examples, Euclidean- (affine-) equivalent point configurations may or may not belong to the same Wyckoff position. Consequently, normalizers also define equivalence relations on Wyckoff positions:

Two *Wyckoff positions* of a space group $\mathcal{G}$ are called *Euclidean-* or $\mathcal{N}_{\mathcal{E}}$-equivalent (*affine-* or $\mathcal{N}_{\mathcal{A}}$-*equivalent*) if their point configurations are mapped onto each other by the Euclidean (affine) normalizer of $\mathcal{G}$.

Euclidean-equivalent Wyckoff positions are important for the description or comparison of crystal structures in terms of atomic coordinates. Affine-equivalent Wyckoff positions result in *Wyckoff sets* (*cf.* Sections 1.4.4 and 3.4.1.2) and form the necessary basis for the *definition of lattice complexes.* All site-symmetry groups corresponding to equivalent Wyckoff positions are conjugate in the respective normalizer.

Table 3.5.2.6
Affine normalizers of the triclinic and monoclinic space groups

Space group $\mathcal{G}$		Matrix–column pairs in Table 3.5.2.7
No.	Hermann–Mauguin symbol	
1	$P1$	$\boldsymbol{M}_1, \boldsymbol{v}_1$
2	$P\bar{1}$	$\boldsymbol{M}_1, \boldsymbol{v}_2$
3	$P121$	$\boldsymbol{M}_2, \boldsymbol{v}_3$
3	$P112$	$\boldsymbol{M}_3, \boldsymbol{v}_4$
4	$P12_11$	$\boldsymbol{M}_2, \boldsymbol{v}_3$
4	$P112_1$	$\boldsymbol{M}_3, \boldsymbol{v}_4$
5	$C121$	$\boldsymbol{M}_4, \boldsymbol{v}_3$
5	$A121$	$\boldsymbol{M}_5, \boldsymbol{v}_3$
5	$I121$	$\boldsymbol{M}_6, \boldsymbol{v}_3$; $\boldsymbol{M}_7, \boldsymbol{v}_3$
5	$A112$	$\boldsymbol{M}_8, \boldsymbol{v}_4$
5	$B112$	$\boldsymbol{M}_9, \boldsymbol{v}_4$
5	$I112$	$\boldsymbol{M}_{10}, \boldsymbol{v}_4$; $\boldsymbol{M}_{11}, \boldsymbol{v}_4$
6	$P1m1$	$\boldsymbol{M}_2, \boldsymbol{v}_5$
6	$P11m$	$\boldsymbol{M}_3, \boldsymbol{v}_6$
7	$P1c1$	$\boldsymbol{M}_5, \boldsymbol{v}_5$
7	$P1n1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_5$
7	$P1a1$	$\boldsymbol{M}_4, \boldsymbol{v}_5$
7	$P11a$	$\boldsymbol{M}_9, \boldsymbol{v}_6$
7	$P11n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_6$
7	$P11b$	$\boldsymbol{M}_8, \boldsymbol{v}_6$
8	$C1m1$	$\boldsymbol{M}_4, \boldsymbol{v}_5$
8	$A1m1$	$\boldsymbol{M}_5, \boldsymbol{v}_5$
8	$I1m1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_5$
8	$A11m$	$\boldsymbol{M}_8, \boldsymbol{v}_6$
8	$B11m$	$\boldsymbol{M}_9, \boldsymbol{v}_6$
8	$I11m$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_6$
9	$C1c1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_{12}, \boldsymbol{v}_7$
9	$A1n1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_{13}, \boldsymbol{v}_7$
9	$I1a1$	$\boldsymbol{M}_6, \boldsymbol{v}_5$; $\boldsymbol{M}_7, \boldsymbol{v}_7$
9	$A11a$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{14}, \boldsymbol{v}_8$
9	$B11n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{15}, \boldsymbol{v}_8$
9	$I11b$	$\boldsymbol{M}_{10}, \boldsymbol{v}_6$; $\boldsymbol{M}_{11}, \boldsymbol{v}_8$
10	$P12/m1$	$\boldsymbol{M}_2, \boldsymbol{v}_2$
10	$P112/m$	$\boldsymbol{M}_3, \boldsymbol{v}_2$
11	$P12_1/m1$	$\boldsymbol{M}_2, \boldsymbol{v}_2$
11	$P112_1/m$	$\boldsymbol{M}_3, \boldsymbol{v}_2$
12	$C12/m1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
12	$A12/m1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
12	$I12/m1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
12	$A112/m$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
12	$B112/m$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
12	$I112/m$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
13	$P12/c1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
13	$P12/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
13	$P12/a1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
13	$P112/a$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
13	$P112/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
13	$P112/b$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
14	$P12_1/c1$	$\boldsymbol{M}_5, \boldsymbol{v}_2$
14	$P12_1/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_2$
14	$P12_1/a1$	$\boldsymbol{M}_4, \boldsymbol{v}_2$
14	$P112_1/a$	$\boldsymbol{M}_9, \boldsymbol{v}_2$
14	$P112_1/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_2$
14	$P112_1/b$	$\boldsymbol{M}_8, \boldsymbol{v}_2$
15	$C12/c1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_{12}, \boldsymbol{v}_9$
15	$A12/n1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_{13}, \boldsymbol{v}_{10}$
15	$I12/a1$	$\boldsymbol{M}_6, \boldsymbol{v}_2$; $\boldsymbol{M}_7, \boldsymbol{v}_{11}$
15	$A112/a$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{14}, \boldsymbol{v}_{10}$
15	$B112/n$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{15}, \boldsymbol{v}_{12}$
15	$I112/b$	$\boldsymbol{M}_{10}, \boldsymbol{v}_2$; $\boldsymbol{M}_{11}, \boldsymbol{v}_{11}$

Table 3.5.2.7
Matrices and columns used in Table 3.5.2.6 for the description of the affine normalizers of monoclinic and triclinic space groups

n, g and u represent integer, even and odd numbers, respectively, r, s and t real numbers. For all matrices, $\det(\boldsymbol{M}_i) = \pm 1$ must hold.

$$\boldsymbol{M}_1 = \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} \quad \boldsymbol{M}_2 = \begin{pmatrix} n_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & n_{33} \end{pmatrix} \quad \boldsymbol{M}_3 = \begin{pmatrix} n_{11} & n_{12} & 0 \\ n_{21} & n_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_4 = \begin{pmatrix} u_{11} & 0 & n_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_5 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ n_{31} & 0 & u_{33} \end{pmatrix}$$

$$\boldsymbol{M}_6 = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_7 = \begin{pmatrix} g_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & g_{33} \end{pmatrix} \quad \boldsymbol{M}_8 = \begin{pmatrix} u_{11} & g_{12} & 0 \\ n_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_9 = \begin{pmatrix} u_{11} & n_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{10} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$$

$$\boldsymbol{M}_{11} = \begin{pmatrix} g_{11} & u_{12} & 0 \\ u_{21} & g_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{12} = \begin{pmatrix} u_{11} & 0 & u_{13} \\ 0 & \pm 1 & 0 \\ g_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_{13} = \begin{pmatrix} u_{11} & 0 & g_{13} \\ 0 & \pm 1 & 0 \\ u_{31} & 0 & u_{33} \end{pmatrix} \quad \boldsymbol{M}_{14} = \begin{pmatrix} u_{11} & g_{12} & 0 \\ u_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \quad \boldsymbol{M}_{15} = \begin{pmatrix} u_{11} & u_{12} & 0 \\ g_{21} & u_{22} & 0 \\ 0 & 0 & \pm 1 \end{pmatrix}$$

$$\boldsymbol{v}_1 = \begin{pmatrix} r \\ s \\ t \end{pmatrix} \quad \boldsymbol{v}_2 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_3 = \begin{pmatrix} \frac{1}{2}n_1 \\ s \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_4 = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{2}n_2 \\ t \end{pmatrix} \quad \boldsymbol{v}_5 = \begin{pmatrix} r \\ \frac{1}{2}n_2 \\ t \end{pmatrix}$$

$$\boldsymbol{v}_6 = \begin{pmatrix} r \\ s \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_7 = \begin{pmatrix} r \\ \frac{1}{4}u_2 \\ t \end{pmatrix} \quad \boldsymbol{v}_8 = \begin{pmatrix} r \\ s \\ \frac{1}{4}u_3 \end{pmatrix} \quad \boldsymbol{v}_9 = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{2}n_3 \end{pmatrix} \quad \boldsymbol{v}_{10} = \begin{pmatrix} \frac{1}{2}n_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix}$$

$$\boldsymbol{v}_{11} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{4}u_2 \\ \frac{1}{4}u_3 \end{pmatrix} \quad \boldsymbol{v}_{12} = \begin{pmatrix} \frac{1}{4}u_1 \\ \frac{1}{2}n_2 \\ \frac{1}{4}u_3 \end{pmatrix}$$

Examples

The Euclidean and affine normalizer of $I\bar{4}m2$ is $I4/mmm$ ($\frac{1}{2}\mathbf{a}-\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c}$). It maps the point configurations $2a$ 0, 0, 0, $2b$ 0, 0, $\frac{1}{2}$, $2c$ 0, $\frac{1}{2}$, $\frac{1}{4}$ and $2d$ 0, $\frac{1}{2}$, $\frac{3}{4}$ (body-centred tetragonal lattices) onto each other. Accordingly, Wyckoff positions *a* to *d* are affine-equivalent and together form a Wyckoff set. Analogous point configurations exist in subgroup $P\bar{4}n2$ of $I\bar{4}m2$ (again Wyckoff positions *a* to *d*). The Euclidean and affine normalizer of $P\bar{4}n2$, however, is $P4/mmm$ ($\frac{1}{2}\mathbf{a}-\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{a}+\frac{1}{2}\mathbf{b},\frac{1}{2}\mathbf{c}$), not containing $t(\frac{1}{2},0,\frac{1}{4})$. Therefore, Wyckoff positions *a* and *b* form one Wyckoff set, *c* and *d* a different one. This is also reflected in the site-symmetry groups $\bar{4}$.. and 2.22.

The existence of Euclidean-equivalent point configurations results in different but *equivalent descriptions of crystal structures* (exception: crystal structures with symmetry $Im\bar{3}m$ or $Ia\bar{3}d$). All such equivalent descriptions are derived by applying the additional generators of the Euclidean normalizer of the space group $\mathcal{G}$ to all point configurations of the original description. Since an adequate description of a crystal structure always displays the full symmetry group of that structure, the number of equivalent descriptions must equal the index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example

Ag_3PO_4 crystallizes with symmetry $P\bar{4}3n$ (*cf.* Masse *et al.*, 1976): P at $2a$ 0, 0, 0, Ag at $6d$ $\frac{1}{4}$, 0, $\frac{1}{2}$ and O at $8e$ x,x,x with $x=0.1486$. $\mathcal{N}_{\mathcal{E}}(P\bar{4}3n)=Im\bar{3}m$ with index 4 gives rise to three additional equivalent descriptions: $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ yields P at $2a$ 0, 0, 0, Ag at $6c$ $\frac{1}{4}$, $\frac{1}{2}$, 0 and O at $8e$ x,x,x with $x=0.1486$; inversion through the origin results in P at $2a$ 0, 0, 0, Ag at $6d$ $\frac{1}{4}$, 0, $\frac{1}{2}$, O at $8e$ x,x,x with $x=-0.1486$ and in P at $2a$ 0, 0, 0, Ag at $6c$ $\frac{1}{4}$, $\frac{1}{2}$, 0 and O at $8e$ x,x,x with $x=-0.1486$. Although the phosphorus configuration is the same for all descriptions and the silver and oxygen atoms refer to only two configurations each, their combinations result in a total of four different equivalent descriptions of the structure.

If the Euclidean normalizer of a space group contains continuous translations, each crystal structure with that symmetry refers to an infinite set of equivalent descriptions. This set may be subdivided into a finite number of subsets in such a way that the descriptions of each subset vary according to the continuous translations. The number of these subsets is given by the product of the finite factors listed in the last column of Tables 3.5.2.3, 3.5.2.4 and 3.5.2.5.

Example

The tetragonal form of $BaTiO_3$ has been described in space group $P4mm$ (*cf. e.g.* Buttner & Maslen, 1992): Ba at $1a$ 0, 0, z with $z=0$, Ti at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=0.482$, O1 at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=0.016$, and O2 at $2c$ $\frac{1}{2}$, 0, z with $z=0.515$. $\mathcal{N}_{\mathcal{E}}(P4mm)=P^{1}4/mmm$ ($\frac{1}{2}(\mathbf{a}-\mathbf{b}),\frac{1}{2}(\mathbf{a}+\mathbf{b}),\varepsilon\mathbf{c}$) gives rise to $(2\cdot\infty)\cdot 2\cdot 1$ equivalent descriptions of this structure. The continuous translation with vector $(0,0,t)$ yields a first infinite subset of equivalent descriptions: Ba at $1a$ 0, 0, z with $z=t$, Ti at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=0.482+t$, O1 at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=0.016+t$, and O2 at $2c$ $\frac{1}{2}$, 0, z with $z=0.515+t$. The translation with vector $(\frac{1}{2},\frac{1}{2},0)$ generates a second infinite subset: Ba at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=t$, Ti at $1a$ 0, 0, z with $z=0.482+t$, O1 at $1a$ 0, 0, z with $z=0.016+t$, and O2 at $2c$ $\frac{1}{2}$, 0, z with $z=0.515+t$. Inversion through the origin causes two further infinite subsets of equivalent coordinate descriptions of $BaTiO_3$: first, Ba at $1a$ 0, 0, z with $z=t$, Ti at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=0.518+t$, O1 at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=-0.016+t$, and O2 at $2c$ $\frac{1}{2}$, 0, z with $z=0.485+t$; second, Ba at $1b$ $\frac{1}{2}$, $\frac{1}{2}$, z with $z=t$, Ti at $1a$ 0, 0, z with $z=0.518+t$, O1 at $1a$ 0, 0, z with $z=-0.016+t$, and O2 at $2c$ $\frac{1}{2}$, 0, z with $z=0.485+t$.

For any chiral crystal structure two variants with opposite handedness exist and the corresponding symmetry group $\mathcal{G}$ is a Sohncke space group, *i.e.* a group without improper motions. Two cases should be distinguished:

(1) $\mathcal{G}$ is an achiral space group. Then its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ contains improper motions and interchanges the coordinate descriptions of crystals with different handedness. To obtain equivalent descriptions of the chiral crystal structure without inverting the chirality, only the additional generators of the chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ should be used.

(2) $\mathcal{G}$ belongs to a pair of chiral space groups. Then its Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ consists only of proper motions, *i.e.* it likewise is a Sohncke space group. In that case, the symmetry groups of enantiomorphic crystals are enantimorphic space groups and, therefore, their coordinate descriptions cannot be mapped onto one another by symmetry operations from $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

Example for case (1)

The phosphorus atoms of NaP form helical chains with (slightly distorted) symmetry $\not{p}4_322$ (rod group of the molecules, not imposed by the space group; Schnering & Hönle, 1979). The chains wind round 2_1 axes parallel to **b** in the space group $\mathcal{G}=P2_12_12_1$. The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is $Pmmm$ with halved basis vectors (Table 3.5.2.4); the chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is its noncentrosymmetric subgroup $P222$. The index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ is 16 and shows the existence of 16 equivalent descriptions, namely of 8 enantiomorphic pairs. The index of $\mathcal{G}$ in $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is 8. This corresponds to eight equivalent coordinate sets which can be obtained by application of the translations 0, 0, 0; $\frac{1}{2}$, 0, 0; 0, $\frac{1}{2}$, 0; 0, 0, $\frac{1}{2}$; $\frac{1}{2}$, $\frac{1}{2}$, 0; $\frac{1}{2}$, 0, $\frac{1}{2}$; 0, $\frac{1}{2}$, $\frac{1}{2}$ and $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$. The remaining eight, with the opposite chirality, result from the same translations in addition to an inversion. The inversion converts the left-handed $\not{p}4_322$ helices to the enantiomorphic right-handed $\not{p}4_122$ helices. The chirality is a property of the polymeric $(P^{-})_{\infty}$ ions. The space group $P2_12_12_1$ itself is not chiral, but it contains no symmetry operations that interconvert the enantiomeric ions; it is a Sohncke space group. The non-chiral space group $P2_12_12_1$ is compatible with either of the enantiomorphic forms of NaP.

Example for case (2)

Low-temperature quartz crystallizes either with symmetry $\mathcal{G}_1=P3_121$ (left-handed quartz) or $\mathcal{G}_2=P3_221$ (right-handed), which is a pair of enantiomorphic (chiral) space groups. Their Euclidean normalizers also form a pair of enantiomorphic space groups, namely $\mathcal{N}_{\mathcal{E}}(\mathcal{G}_1)=\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}_1)=P6_222$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G}_2)=\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}_2)=P6_422$ with halved **c** vectors; they consist only of proper motions and thus are chirality preserving. The index of $P3_121$ in its Euclidean normalizer is 4, which means that there are four equivalent descriptions for left-handed quartz. They are mapped onto each other by the translation 0, 0, $\frac{1}{2}$ and the rotation $-x,-y,z$ (Table 3.5.2.5). The same applies to right-handed quartz. Left-handed quartz

cannot be mapped onto right-handed quartz by the Euclidean normalizer. The four equivalent descriptions retain the chirality.

More details on Euclidean-equivalent point configurations and descriptions of crystal structures have been given by Fischer & Koch (1983) and Koch & Fischer (2006).

3.5.3.3. Equivalent lists of structure factors

All the different but equivalent descriptions of a crystal structure refer to different but equivalent lists of structure factors. These lists contain the same moduli of the structure factors $|F(\boldsymbol{h})|$, but they differ in their indices $\boldsymbol{h} = (h, k, l)$ and phases $\varphi(\boldsymbol{h})$.

In the previous section, the unit cell (basis and origin) of a space group $\mathcal{G}$ has been considered fixed, whereas the crystal structure or its enantiomorph was embedded into the pattern of symmetry elements at different but equivalent locations. In the present context, however, it is advantageous to regard the crystal structure as being fixed and to let $\mathcal{N}_\mathcal{E}(\mathcal{G})$ transform the basis and the origin with respect to which the crystal structure is described. This matches the usual approach to resolve the ambiguities in direct methods by fixing the origin and the absolute structure.

Each matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ representing an element of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ describes a unit-cell transformation of $\mathcal{G}$. According to Section 1.5.2 the following equations hold:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}'), = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}, \quad \begin{pmatrix} \mathbf{a}^{*\prime} \\ \mathbf{b}^{*\prime} \\ \mathbf{c}^{*\prime} \end{pmatrix} = \boldsymbol{P}^{-1} \begin{pmatrix} \mathbf{a}^{*} \\ \mathbf{b}^{*} \\ \mathbf{c}^{*} \end{pmatrix}, \quad \boldsymbol{h}' = \boldsymbol{h}\boldsymbol{P}.$$

As a consequence, the phase $\varphi(\boldsymbol{h})$ of a given structure factor also changes into $\varphi'(\boldsymbol{h}') = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{h}\boldsymbol{p}$.

Similar to equivalent descriptions of a crystal structure, it is possible to derive all equivalent lists of structure factors: The additional generators of $\mathcal{K}(\mathcal{G})$ are pure translations that leave the indices $\boldsymbol{h}$ of all structure factors unchanged but transform their phases according to $\varphi'(\boldsymbol{h}) = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{h}\boldsymbol{p}$. Therefore, the origin for the description of the crystal structure may be fixed by appropriate restrictions of some phases. The number of these phases equals the number of additional generators of $\mathcal{K}(\mathcal{G})$, given in Tables 3.5.2.3, 3.5.2.4 or 3.5.2.5. These generators [together with the inversion that generates $\mathcal{L}(\mathcal{G})$, if present] also determine the parity classes of the structure factors and the ranges for the phase restrictions.

The inversion that generates $\mathcal{L}(\mathcal{G})$ changes the handedness of the coordinate system in direct space and in reciprocal space and, therefore, gives rise to different absolute crystal structures. The indices of a given structure factor change from $\boldsymbol{h}$ to $\boldsymbol{h}' = -\boldsymbol{h}$, whereas the phase is influenced only if the symmetry centre is not located at 0, 0, 0.

If no anomalous scattering is observed, Friedel's rule holds and the moduli of any two structure factors with indices $\boldsymbol{h}$ and $-\boldsymbol{h}$ are equal. As a consequence, different absolute crystal structures result in lists of structure factors and indices that differ only in their phases. Therefore, one phase may be restricted to an appropriate range of length π to fix the absolute structure. This is not possible if anomalous scattering has been observed.

If $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{N}_\mathcal{E}(\mathcal{G})$, *i.e.* if $\mathcal{G}$ and $\mathcal{N}_\mathcal{E}(\mathcal{G})$ belong to different Laue classes, the further generators of $\mathcal{N}_\mathcal{E}(\mathcal{G})$ always change the orientation of the basis in direct and in reciprocal space. Therefore, the indices of the structure factors are permuted, but their phases are transformed only if $\boldsymbol{p} \neq \boldsymbol{o}$. The choice between these equivalent descriptions of the crystal structure is made when indexing the reflection pattern. In the case of anomalous scattering, the similar choice between the absolute structures is also combined with the indexing procedure.

Table 3.5.3.1
Changes of structure-factor phases for the equivalent descriptions of a crystal structure in *F*222

	$h+k+l=$			
*F*222	$4n$	$4n+2$	$4n+1$	$4n+3$
$t(0,0,0)$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$
$t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi+\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi+\varphi(\boldsymbol{h})$
$t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$
$t(\frac{3}{4},\frac{3}{4},\frac{3}{4})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi+\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi+\varphi(\boldsymbol{h})$
$\bar{1}$ 0, 0, 0	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$
$\bar{1}$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi-\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi-\varphi(\boldsymbol{h})$
$\bar{1}$ $\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$
$\bar{1}$ $\frac{3}{8},\frac{3}{8},\frac{3}{8}$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi-\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi-\varphi(\boldsymbol{h})$

Example

According to Table 3.5.2.4, eight equivalent descriptions exist for each crystal structure with symmetry *F*222. Four of them differ only by an origin shift and the other four are enantiomorphic to the first four. $t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ transforms all phases according to $\varphi'(\boldsymbol{h}) = \varphi(\boldsymbol{h}) - (\pi/2)(h+k+l)$, which gives rise to four parity classes of structure factors: $h+k+l = 4n$, $4n+1$, $4n+2$ and $4n+3$ (n integer). As $t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ generates all additional translations of $\mathcal{K}(F222)$, restriction of one phase $\varphi(\boldsymbol{h}_1)$ to a range of length $\pi/2$ fixes the origin. Restriction of a second phase $\varphi(\boldsymbol{h}_2)$ to an appropriately chosen range of length π discriminates between pairs of enantiomorphic descriptions in the absence of anomalous scattering. For inversion through the origin $\bar{1}$ 0, 0, 0, the corresponding change of phases is $\varphi'(\boldsymbol{h}) = -\varphi(\boldsymbol{h})$. Table 3.5.3.1 shows, for structure factors from all parity classes, how their phases depend on the chosen description of the crystal structure. Only phases from parity classes $h+k+l = 4n+1$ or $4n+3$ determine the origin in a unique way. The phase $\varphi(\boldsymbol{h}_2)$ that fixes the absolute structure may be chosen from any parity class but the appropriate range for its restriction depends on the parity classes of $\varphi(\boldsymbol{h}_1)$ *and* $\varphi(\boldsymbol{h}_2)$ and, moreover, on the range chosen for $\varphi(\boldsymbol{h}_1)$. If, for instance, $\varphi(\boldsymbol{h}_1)$ with $h+k+l = 4n+1$ is restricted to $\pi/2 \leq \varphi(\boldsymbol{h}_1) < \pi$, one of the following restrictions may be chosen for $\varphi(\boldsymbol{h}_2)$: $0 < \varphi(\boldsymbol{h}_2) < \pi$ for $h+k+l = 4n$; $-\pi/2 < \varphi(\boldsymbol{h}_2) < \pi/2$ for $h+k+l = 4n+2$; $-\pi/4 < \varphi(\boldsymbol{h}_2) < 3\pi/4$ for $h+k+l = 4n+1$; $-3\pi/4 < \varphi(\boldsymbol{h}_2) < \pi/4$ for $h+k+l = 4n+3$. If, however, the phase $\varphi(\boldsymbol{h}_1)$ of the same first reflection was restricted to $-\pi/4 \leq \varphi(\boldsymbol{h}_1) < 3\pi/4$, the possible restrictions for the second phase change to: $0 < \varphi(\boldsymbol{h}_2) < \pi$ for $h+k+l = 4n$ or $4n+2$; $-\pi/2 < \varphi(\boldsymbol{h}_2) < \pi/2$ for $h+k+l = 4n+1$ or $4n+3$ (for further details, *cf.* Koch, 1986).

3.5.3.4. Euclidean- and affine-equivalent sub- and supergroups

The Euclidean or affine normalizer of a space group $\mathcal{G}$ maps any subgroup or supergroup of $\mathcal{G}$ either onto itself or onto another subgroup or supergroup of $\mathcal{G}$. Accordingly, these normalizers define equivalence relationships on the sets of subgroups and supergroups of $\mathcal{G}$ (Koch, 1984*b*):

Two *subgroups* or *supergroups* of a space group $\mathcal{G}$ are called *Euclidean-* or $\mathcal{N}_\mathcal{E}$*-equivalent* (*affine-* or $\mathcal{N}_\mathcal{A}$*-equivalent*) if they are mapped onto each other by an element of the Euclidean (affine)

normalizer of $\mathcal{G}$, *i.e.* if they are conjugate subgroups of the Euclidean (affine) normalizer.

In the following, the term 'equivalent subgroups (supergroups)' is used if a statement is true for Euclidean-equivalent *and* affine-equivalent subgroups (supergroups), and $\mathcal{N}(\mathcal{G})$ is used to designate the Euclidean as well as the affine normalizer.

The knowledge of Euclidean-equivalent subgroups is necessary in connection with the possible deformations of a crystal structure due to symmetry reduction. Affine-equivalent subgroups play an important role for the derivation and classification of black-and-white groups (magnetic groups) and of colour groups (*cf.* for example Schwarzenberger, 1984). Information on equivalent supergroups is useful for the determination of the idealized type of a crystal structure.

For any pair of space groups $\mathcal{G}$ and $\mathcal{H}$ with $\mathcal{H} < \mathcal{G}$, the relation between the two normalizers $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{H})$ controls the subgroups of $\mathcal{G}$ that are equivalent to $\mathcal{H}$ and the supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. The intersection group of both normalizers, $\mathcal{M}(\mathcal{G}, \mathcal{H}) = \mathcal{N}(\mathcal{G}) \cap \mathcal{N}(\mathcal{H}) \geq \mathcal{H}$ may or may not coincide with $\mathcal{N}(\mathcal{G})$ and/or with $\mathcal{N}(\mathcal{H})$. The following two statements hold generally:

(i) The index i_g of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ equals the number of subgroups of $\mathcal{G}$ which are equivalent to $\mathcal{H}$. Each coset of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ maps $\mathcal{H}$ onto another equivalent subgroup of $\mathcal{G}$.

(ii) The index i_h of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ equals the number of supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. Each coset of $\mathcal{M}(\mathcal{G}, \mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ maps $\mathcal{G}$ onto another equivalent supergroup of $\mathcal{H}$.

Equivalent subgroups are *conjugate* in $\mathcal{G}$ if and only if $\mathcal{G} \cap \mathcal{N}(\mathcal{H}) \neq \mathcal{G}$. In this case, $\mathcal{G}$ contains elements not belonging to $\mathcal{N}(\mathcal{H})$ and the cosets of $\mathcal{G} \cap \mathcal{N}(\mathcal{H})$ in $\mathcal{G}$ refer to the different conjugate subgroups.

Examples

(1) $\mathcal{G} = Cmmm$ has four monoclinic subgroups of type $P2/m$ with the same orthorhombic metric and the same basis as $Cmmm$: $\mathcal{H}_1 = P2/m11$, $\mathcal{H}_2 = P12/m1$, $\mathcal{H}_3 = P112/m$ ($\bar{1}$ at $0, 0, 0$), $\mathcal{H}_4 = P112/m$ ($\bar{1}$ at $\frac{1}{4}, \frac{1}{4}, 0$). According to Table 3.5.2.4, the Euclidean normalizer of $\mathcal{G}$ is $Pmmm$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$). Because of the orthorhombic metric of all four subgroups, their Euclidean normalizers $\mathcal{N}_\mathcal{E}(\mathcal{H}_1)$, $\mathcal{N}_\mathcal{E}(\mathcal{H}_2)$, $\mathcal{N}_\mathcal{E}(\mathcal{H}_3)$ and $\mathcal{N}_\mathcal{E}(\mathcal{H}_4)$ are enhanced in comparison with the general case and coincide with $\mathcal{N}_\mathcal{E}(\mathcal{G})$. Hence, no two of the four subgroups are Euclidean-equivalent.

(2) $\mathcal{G} = I\bar{4}m2$ ($\mathbf{a}, \mathbf{b}, \mathbf{c}$), $\mathcal{H} = P\bar{4}$ ($\mathbf{a}, \mathbf{b}, \mathbf{c}$).
$\mathcal{N}(\mathcal{G}) = I4/mmm$ ($\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) is a supergroup of index 2 of $\mathcal{N}(\mathcal{H}) = P4/mmm$ ($\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) = $\mathcal{M}(I\bar{4}m2, P\bar{4})$. Therefore, $I\bar{4}m2$ has two equivalent subgroups $P\bar{4}$ that are mapped onto one another by a centring translation of $\mathcal{N}(\mathcal{G})$, *e.g.* by $t(0, \frac{1}{2}, \frac{1}{4})$. Both subgroups are not conjugate in $I\bar{4}m2$ because $\mathcal{G} \cap \mathcal{N}(\mathcal{H})$ equals $\mathcal{G}$. As $\mathcal{N}(\mathcal{H})$ coincides with $\mathcal{M}(\mathcal{G}, \mathcal{H})$, no further supergroups of $P\bar{4}$ equivalent to $I\bar{4}m2$ exist.

(3) $\mathcal{G} = Fm\bar{3}$ ($\mathbf{a}, \mathbf{b}, \mathbf{c}$), $\mathcal{H} = F23$ ($\mathbf{a}, \mathbf{b}, \mathbf{c}$).
$\mathcal{N}(\mathcal{H}) = Im\bar{3}m$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) is a supergroup of index 2 of $\mathcal{N}(\mathcal{G}) = Pm\bar{3}m$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) = $\mathcal{M}(Fm\bar{3}, F23)$. Therefore, $F23$ has two equivalent supergroups $Fm\bar{3}$ that differ in their locations with site symmetry $m\bar{3}$ by a centring translation of $Im\bar{3}m$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$), *e.g.* by $t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. As $\mathcal{N}(\mathcal{G})$ coincides with $\mathcal{M}(\mathcal{G}, \mathcal{H})$, no further subgroups of $Fm\bar{3}$ equivalent to $F23$ exist.

(4) $\mathcal{G} = Pmma$ ($\mathbf{a}, \mathbf{b}, \mathbf{c}$), $\mathcal{H} = Pmmn$ ($\mathbf{a}, 2\mathbf{b}, \mathbf{c}$).
The intersection of $\mathcal{N}_\mathcal{A}(Pmma) = Pmmm$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) and $\mathcal{N}_\mathcal{A}(Pmmn) = P4/mmm$ ($\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$) is the group $\mathcal{M}(Pmma, Pmmn) = Pmmm$ ($\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c}$), which is a proper subgroup of both normalizers. As i_g equals 2, $Pmma$ has two affine-equivalent subgroups of type $Pmmn$ that are mapped onto each other by the additional translation $t(0, \frac{1}{2}, 0)$ of the normalizer of $\mathcal{G}$. As i_h also equals 2, $Pmmn$ has two affine-equivalent supergroups, $Pmma$ and $Pmmb$, that are mapped onto each other, *e.g.* by the affine 'reflection' at a diagonal 'mirror plane' of $\mathcal{N}_\mathcal{A}(\mathcal{H})$.

3.5.3.5. Reduction of the parameter regions to be considered for geometrical studies of point configurations

Each point configuration with space-group symmetry $\mathcal{G}$ may be described by its metrical and coordinate parameters. To cover all point configurations belonging to a certain space-group type exactly once, the metrical parameters of $\mathcal{G}$ have to be varied without restrictions, whereas the coordinate parameters x, y and z must be restricted to one asymmetric unit of $\mathcal{G}$. For the study of the geometrical properties of point configurations (*e.g.* sphere-packing conditions or types of Dirichlet domains *etc.*), the Euclidean normalizers (*cf. e.g.* Laves, 1931; Fischer, 1971, 1991; Koch, 1984*a*) as well as the affine normalizers (*cf.* Fischer, 1968) of the space groups allow a further reduction of the parameter regions that have to be considered.

Examples

(1) $\mathcal{G} = P4/m$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$: A geometrical consideration may be restricted to one asymmetric unit of $\mathcal{N}_\mathcal{E}(\mathcal{G}) = \mathcal{N}_\mathcal{A}(\mathcal{G}) = P4/mmm$ ($\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$), *i.e.* to the region $0 \leq x \leq \frac{1}{2}$, $y \leq \min(x, \frac{1}{2} - x)$, $0 \leq z \leq \frac{1}{4}$. All metrical parameters are unrestricted.

(2) $\mathcal{G} = P4$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \leq z < 1$: The normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G}) = \mathcal{N}_\mathcal{A}(\mathcal{G}) = P^1 4/mmm$ ($\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c}$) restricts the parameter region to be considered to $0 \leq x \leq \frac{1}{2}$, $y \leq \min(x, \frac{1}{2} - x)$, $z = 0$. Again, no restriction exists for the metrical parameters.

(3) $\mathcal{G} = Pmmm$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 \leq y \leq \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$: The Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G}) = Pmmm$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) reduces the parameter region to be considered to $0 \leq x \leq \frac{1}{4}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z \leq \frac{1}{4}$. All metrical parameters are unrestricted. The affine normalizer $\mathcal{N}_\mathcal{A}(\mathcal{G}) = Pm\bar{3}m$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) enables a further reduction of the parameter region that has to be studied. For this, two different possibilities exist:
(i) the metrical parameters remain unrestricted but the coordinate parameters are limited to one asymmetric unit of $\mathcal{N}_\mathcal{A}(\mathcal{G})$, *i.e.* to $0 \leq x \leq \frac{1}{4}$, $0 \leq y \leq x$, $0 \leq z \leq y$;
(ii) the coordinate parameters are not further restricted, but the metrical parameters have to obey *e.g.* the relation $a \leq b \leq c$, *i.e.* $a/c \leq b/c \leq 1$.

(4) $\mathcal{G} = P112/m$ with asymmetric unit $0 \leq x < 1$, $0 \leq y \leq \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$. The Euclidean normalizer $\mathcal{N}_\mathcal{E}(\mathcal{G}) = P112/m$ ($\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}$) reduces the region that has to be considered for the coordinate parameters to $0 \leq x < \frac{1}{2}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z \leq \frac{1}{4}$, but it does not impose restrictions on the metrical parameters. These may be restricted, however, to the range $a/b \leq 1$ and $0 \leq 2\cos\gamma \leq -a/b$ (as shown in Fig. 3.5.2.1) by means of the affine normalizer $\mathcal{N}_\mathcal{A}(P112/m)$.

3.5.4. Normalizers of point groups

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Normalizers with respect to the Euclidean or affine group may be defined for any group of isometries (*cf.* Gubler, 1982*a*,*b*). For a point group, however, it seems inadequate to use a supergroup that contains transformations that do not map a fixed point of that point group onto itself. Appropriate supergroups for the definition of normalizers of point groups are the full isometry groups of the sphere, $m\overline{\infty}$, and of the circle, ∞m, in three-dimensional and two-dimensional space (*cf.* Galiulin, 1978).

These normalizers are listed in Tables 3.5.4.1 and 3.5.4.2. It has to be noticed that the normalizer of a crystallographic point group may contain continuous rotations, *i.e.* rotations with infinitesimal rotation angle, or noncrystallographic rotations (∞m; $m\overline{\infty}$, ∞/mm, $8mm$, $12mm$; $8/mmm$, $12/mmm$). In analogy to space groups, these normalizers define equivalence relationships on the 'Wyckoff positions' of the point groups (*cf.* Sections 3.2.3 and 3.2.4). They give also the relation between the different but equivalent morphological descriptions of a crystal.

Table 3.5.4.1
Normalizers of the two-dimensional point groups with respect to the full isometry group of the circle

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 3.2.1.5. The letter n represents an arbitrary integer; $(2n)$ represents an even number.

Normalizer	Point groups
∞m	1, 2, 4, 3, 6
$12mm$	$6mm$
$8mm$	$4mm$
$6mm$	$3m$
$4mm$	$2mm$
$2mm$	m
∞m	n, ∞, ∞m
$(2n)mm$	nmm, nm

Table 3.5.4.2
Normalizers of the three-dimensional point groups with respect to the full isometry group of the sphere

The upper part refers to the crystallographic, the lower part to the noncrystallographic point groups as listed in Table 3.2.1.6. The letter n represents an arbitrary integer; $(2n)$ represents an even number.

Normalizer	Point groups
$m\overline{\infty}$	1, $\overline{1}$
$m\overline{3}m$	222, mmm, 23, $m\overline{3}$, 432, $\overline{4}3m$, $m\overline{3}m$
∞/mm	2, m, $2/m$, 4, $\overline{4}$, $4/m$, 3, $\overline{3}$, 6, $\overline{6}$, $6/m$
$12/mmm$	622, $6mm$, $6/mmm$
$8/mmm$	422, $4mm$, $4/mmm$
$6/mmm$	32, $3m$, $\overline{3}m$, $\overline{6}2m$
$4/mmm$	$mm2$, $\overline{4}2m$
$m\overline{\infty}$	2∞, $m\overline{\infty}$
$m\overline{35}$	235, $m\overline{35}$
∞/mm	n, $\overline{n}$, n/m, ∞, ∞/m, $\infty 2$, ∞m, ∞/mm
$(2n)/mmm$	$n22$, nmm, n/mmm, $n2$, nm, $\overline{n}m$
n/mmm	$\overline{n}2m$

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3.6. Magnetic subperiodic groups and magnetic space groups

D. B. Litvin

3.6.1. Introduction

The *magnetic subperiodic groups* in the title refer to generalizations of the crystallographic subperiodic groups, *i.e.* frieze groups (two-dimensional groups with one-dimensional translations), crystallographic rod groups (three-dimensional groups with one-dimensional translations) and layer groups (three-dimensional groups with two-dimensional translations). There are seven frieze-group types, 75 rod-group types and 80 layer-group types, see *International Tables for Crystallography*, Volume E, *Subperiodic Groups* (2010; abbreviated as *IT* E). The magnetic *space groups* refer to generalizations of the one-, two- and three-dimensional crystallographic space groups, n-dimensional groups with n-dimensional translations. There are two one-dimensional space-group types, 17 two-dimensional space-group types and 230 three-dimensional space-group types, see Part 2 of the present volume (*IT* A).

Generalizations of the crystallographic groups began with the introduction of an operation of 'change in colour' and the 'two-colour' (black and white, antisymmetry) crystallographic point groups (Heesch, 1930; Shubnikov, 1945; Shubnikov *et al.*, 1964). Subperiodic groups and space groups were also extended into two-colour groups. Two-colour subperiodic groups consist of 31 two-colour frieze-group types (Belov, 1956*a*,*b*), 394 two-colour rod-group types (Shubnikov, 1959*a*,*b*; Neronova & Belov, 1961*a*,*b*; Galyarski & Zamorzaev, 1965*a*,*b*) and 528 two-colour layer-group types (Neronova & Belov, 1961*a*,*b*; Palistrant & Zamorzaev, 1964*a*,*b*). Of the two-colour space groups, there are seven two-colour one-dimensional space-group types (Neronova & Belov, 1961*a*,*b*), 80 two-colour two-dimensional space-group types (Heesch, 1929; Cochran, 1952) and 1651 two-colour three-dimensional space-group types (Zamorzaev, 1953, 1957*a*,*b*; Belov *et al.*, 1957). See also Zamorzaev (1976), Shubnikov & Koptsik (1974), Koptsik (1966, 1967), and Zamorzaev & Palistrant (1980). [Extensive listings of references on colour symmetry, magnetic symmetry and related topics can be found in the books by Shubnikov *et al.* (1964), Shubnikov & Koptsik (1974), and Opechowski (1986).]

The so-called *magnetic groups*, groups to describe the symmetry of spin arrangements, were introduced by Landau & Lifschitz (1951, 1957) by re-interpreting the operation of 'change in colour' in two-colour crystallographic groups as 'time inversion'. This chapter introduces the structure, properties and symbols of *magnetic* subperiodic groups and *magnetic* space groups as given in the extensive tables by Litvin (2013), which are an extension of the classic tables of properties of the two- and three-dimensional subperiodic groups found in *IT* E and the one-, two- and three-dimensional space groups found in the present volume. A survey of magnetic group types is also presented in Litvin (2013), listing the elements of one representative group in each *reduced superfamily* of the two- and three-dimensional magnetic subperiodic groups and one-, two- and three-dimensional magnetic space groups. Two notations for magnetic groups, the Opechowski–Guccione notation (OG notation) (Guccione, 1963*a*,*b*; Opechowski & Guccione, 1965; Opechowski, 1986) and the Belov–Neronova–Smirnova notation (BNS notation) (Belov *et al.*, 1957) are compared. The maximal subgroups of index ≤ 4 of the magnetic subperiodic groups and magnetic space groups are also given.

3.6.2. Survey of magnetic subperiodic groups and magnetic space groups

We review the concept of a reduced magnetic superfamily (Opechowski, 1986) to provide a classification scheme for magnetic groups. This is used to obtain the survey of the two- and three-dimensional magnetic subperiodic group types and the one-, two- and three-dimensional magnetic space groups given in Litvin (2013). In that survey a specification of a single representative group from each group type is provided.

3.6.2.1. Reduced magnetic superfamilies of magnetic groups

Let $\mathcal{F}$ denote a crystallographic group. The magnetic superfamily of $\mathcal{F}$ consists of the following set of groups:

(1) The group $\mathcal{F}$.
(2) The group $\mathcal{F}1' \equiv \mathcal{F} \times 1'$, the direct product of the group $\mathcal{F}$ and the time-inversion group $1'$, the latter consisting of the identity 1 and time inversion $1'$.
(3) All groups $\mathcal{F}(\mathcal{D}) \equiv \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1' \equiv \mathcal{F} \underline{\times} 1'$, subdirect products of the groups $\mathcal{F}$ and $1'$. $\mathcal{D}$ is a subgroup of index 2 of $\mathcal{F}$. Groups of this kind will also be denoted by $\mathcal{M}$.

The third subset is divided into two subdivisions:

(3*a*) Groups $\mathcal{M}_T$, where $\mathcal{D}$ is an equi-translational (*translationengleiche*) subgroup of $\mathcal{F}$.
(3*b*) Groups $\mathcal{M}_R$, where $\mathcal{D}$ is an equi-class (*klassengleiche*) subgroup of $\mathcal{F}$.[1]

Two magnetic groups $\mathcal{F}_1(\mathcal{D}_1)$ and $\mathcal{F}_2(\mathcal{D}_2)$ are called *equivalent* if there exists an affine transformation that maps $\mathcal{F}_1$ onto $\mathcal{F}_2$ and $\mathcal{D}_1$ onto $\mathcal{D}_2$ (Opechowski, 1986). If only non-equivalent groups $\mathcal{F}(\mathcal{D})$ are included, then the above set of groups is referred to as the reduced magnetic superfamily of $\mathcal{F}$.

Example

We consider the crystallographic point group $\mathcal{F} = 2_x2_y2_z$. The magnetic superfamily of the group $2_x2_y2_z$ consists of five groups: $\mathcal{F} = 2_x2_y2_z$, the group $\mathcal{F}1' = 2_x2_y2_z1'$, and the three groups $\mathcal{F}(\mathcal{D}) = 2_x2_y2_z(2_x)$, $2_x2_y2_z(2_y)$ and $2_x2_y2_z(2_z)$. Since the latter three groups are all equivalent, the reduced magnetic superfamily of the group $\mathcal{F} = 2_x2_y2_z$ consists of only three groups: $2_x2_y2_z$, $2_x2_y2_z1'$, and one of the three groups $2_x2_y2_z(2_x)$, $2_x2_y2_z(2_y)$ and $2_x2_y2_z(2_z)$.

Example

In the reduced magnetic space group superfamily of $\mathcal{F} = Pnn2$ there are five groups: $\mathcal{F} = Pnn2$, $\mathcal{F}1' = Pnn21'$, and three groups $\mathcal{F}(\mathcal{D}) = Pnn2(Pc)$, $Pnn2(P2)$ and $Pnn2(Fdd2)$. The

[1] Replacing time inversion $1'$ by an operation of 'changing two colours', the two-colour groups corresponding to the types 1, 2, 3*a* and 3*b* magnetic groups are known as type I, II, III and IV Shubnikov groups, respectively (Bradley & Cracknell, 1972).

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Table 3.6.2.1
Numbers of types of groups in the reduced magnetic superfamilies of one-, two- and three-dimensional crystallographic point groups, subperiodic groups and space groups

Type of group	$\mathcal{F}$	$\mathcal{F}1'$	$\mathcal{F}(\mathcal{D})$	Total
One-dimensional magnetic point groups	2	2	1	5
Two-dimensional magnetic point groups	10	10	11	31
Three-dimensional magnetic point groups	32	32	58	122
Magnetic frieze groups	7	7	17	31
Magnetic rod groups	75	75	244	394
Magnetic layer groups	80	80	368	528
One-dimensional magnetic space groups	2	2	3	7
Two-dimensional magnetic space groups	17	17	46	80
Three-dimensional magnetic space groups	230	230	1191	1651

groups *Pnn*2(*Pc*) and *Pnn*2(*P*2) are equi-translational magnetic space groups $\mathcal{M}_T$ and *Pnn*2(*Fdd*2) is an equi-class magnetic space group $\mathcal{M}_R$.

A magnetic group has been defined as a symmetry group of a spin arrangement $\mathbf{S}(r)$ (Opechowski, 1986). With this definition, since $1'\mathbf{S}(r) = -\mathbf{S}(r)$, a group $\mathcal{F}1'$ is then not a magnetic group. However, there is not universal agreement on the definition or usage of the term *magnetic group*. Two definitions (Opechowski, 1986) have magnetic groups as symmetry groups of spin arrangements, with one having only groups $\mathcal{F}(\mathcal{D})$, of the three types of groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{F}(\mathcal{D})$, defined as magnetic groups, while a second having both group $\mathcal{F}$ and $\mathcal{F}(\mathcal{D})$ defined as magnetic groups. Here we shall refer to all groups in a magnetic superfamily of a group $\mathcal{F}$ as magnetic groups, while cognizant of the fact that groups $\mathcal{F}1'$ cannot be a symmetry group of a spin arrangement.

3.6.2.2. Survey of magnetic point groups, magnetic subperiodic groups and magnetic space groups

The survey consists of listing the reduced magnetic superfamily of one group from each type of one-, two- and three-dimensional crystallographic point groups, two- and three-dimensional crystallographic subperiodic groups, and one-, two- and three-dimensional space groups (Litvin, 1999, 2001, 2013). The numbers of types of groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{F}(\mathcal{D})$ in the reduced superfamilies of these groups is given in Table 3.6.2.1. The one group from each type, called the *representative group* of that type, is specified by giving a symbol for its translational subgroup and listing a set of coset representatives, called the standard set of coset representatives, of the decomposition of the group with respect to its translational subgroup. The survey provides the following information for each magnetic group type and its associated representative group:

(1) The serial number of the magnetic group type.
(2) A Hermann–Mauguin-like symbol of the magnetic group type which serves also as the symbol of the group type's representative group.
(3) For group types $\mathcal{F}(\mathcal{D})$: The symbol of the group type of the non-primed subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D})$, and the position and orientation of the coordinate system of the representative group $\mathcal{D}$ of the group type $\mathcal{D}$ in the coordinate system of the representative group $\mathcal{F}(\mathcal{D})$.
(4) The standard set of coset representatives of the decomposition of the representative group with respect to its translational subgroup.

Examples of entries in the survey of magnetic groups are given in Table 3.6.2.2. The survey of the three-dimensional magnetic space groups (Litvin, 2001, 2013) was incorporated into the survey of three-dimensional magnetic space groups given by Stokes & Campbell (2009) and the coset representatives can also be found on the Bilbao Crystallographic Server (http://www.cryst.ehu.es; Aroyo *et al.*, 2006).

3.6.2.2.1. Magnetic group type serial number

For each set of magnetic group types, one-, two- and three-dimensional crystallographic magnetic point groups, magnetic subperiodic groups and magnetic space groups, a separate numbering system is used. A three-part composite number $N_1.N_2.N_3$ is given in the first column, see Table 3.6.2.2. N_1 is a sequential number for the group type to which $\mathcal{F}$ belongs. N_2 is a sequential numbering of the magnetic group types of the reduced magnetic superfamily of $\mathcal{F}$. Group types $\mathcal{F}$ always have the assigned number $N_1.1.N_3$, and group types $\mathcal{F}1'$ the assigned number $N_1.2.N_3$. N_3 is a global sequential numbering for each set of magnetic group types. The sequential numbering N_1 for subperiodic groups and space groups follows the numbering in *IT* E and *IT* A, respectively.

3.6.2.2.2. Magnetic group type symbol

A Hermann–Mauguin-like type symbol is given for each magnetic group type in the second column. This symbol denotes both the group type and the representative group of that type. For example, the symbol for the three-dimensional magnetic space-group type 25.4.158 is $Pm'm'2$. This symbol denotes both the group type, which consists of an infinite set of groups, and the representative group $Pm'_xm'_y2_z$. While this representative group may be referred to as 'the group $Pm'm'2$', other groups of this group type, *e.g.* $Pm_{xy}{}'m_{\bar{x}y}{}'2_z$, will always be written with subindices. The representative group of the magnetic group type is defined by its translational subgroup, implied by the first letter in the magnetic group type symbol and defined in Table 1.1 of Litvin (2013), and a given set of coset representatives, called the *standard set of coset representatives*, of the representative group with respect to its translational subgroup.

Only the relative lengths and mutual orientations of the translation vectors of the translational subgroup are given, see Table 1.2 of Litvin (2013). The symmetry directions of symmetry operations represented by characters in the Hermann–Mauguin symbols are implied by the character's position in the symbol and are given in Table 1.3 of Litvin (2013). The standard set of coset representatives are given with respect to an implied coordinate

Table 3.6.2.2
Examples of the format of the survey of magnetic groups of three-dimensional magnetic space-group types

Serial No.	Symbol	Non-primed subgroup of index 2	Standard set of coset representatives			
10.1.49	$P2/m$		$\{1\|0\}$	$\{2_{010}\|0\}$	$\{\bar{1}\|0\}$	$\{m_{010}\|0\}$
10.3.51	$P2'/m$	Pm (0, 0, 0; **a**, **b**, **c**)	$\{1\|0\}$	$\{2_{010}\|0\}$	$\{\bar{1}\|0\}'$	$\{m_{010}\|0\}'$
10.9.57	$P_{2b}2'/m$	$P2_1/m$ (0, $\frac{1}{2}$, 0; **a**, 2**b**, **c**)	$\{1\|0\}$	$\{2_{010}\|0, 1, 0\}$	$\{\bar{1}\|0, 1, 0\}$	$\{m_{010}\|0\}$
50.10.386	$P_{2c}b'a'n'$	$Pnnn$ ($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{2}$; **a**, 2**c**, **b**)	$\{1\|0\}$	$\{2_{100}\|0\}$	$\{2_{010}\|0, 0, 1\}$	$\{2_{001}\|0, 0, 1\}$
			$\{\bar{1}\|\frac{1}{2}, \frac{1}{2}, 1\}$	$\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 1\}$	$\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}$	$\{m_{001}\|\frac{1}{2}, \frac{1}{2}, 0\}$

system. The absolute lengths of translation vectors, the position in space of the origin of the coordinate system and the orientation in that space of the basis vectors of that coordinate system are not explicitly given.

3.6.2.2.3. Standard set of coset representatives

The standard set of coset representatives of each representative group is listed on the right-hand side of the survey of magnetic group types, see *e.g.* Table 3.6.2.2. Each coset in the standard set of coset representatives is given in Seitz notation (Seitz, 1934, 1935*a*,*b*, 1936), *i.e.* $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ or $\{\boldsymbol{R}|\boldsymbol{\tau}\}'$. $\boldsymbol{R}$ denotes a proper or improper rotation (rotation-inversion), $\boldsymbol{\tau}$ a non-primitive translation with respect to the non-primed translational subgroup of the magnetic group, and the prime denotes that $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ is coupled with time inversion. The subindex notation on $\boldsymbol{R}$, denoting the orientation of the proper or improper rotation, is given in Table 1.4 of Litvin (2013). [Note that the Seitz notation used in Litvin (2013) predates and is different from the IUCr standard convention for Seitz symbolism, see Section 1.4.2.2 and Glazer *et al.* (2014).]

3.6.2.2.4. Opechowski–Guccione magnetic group type symbols and the standard set of coset representatives

The specification of the magnetic group type symbol and the standard set of coset representatives of the magnetic group type's representative group is based on the conventions introduced by Opechowski and Guccione (Opechowski & Guccione, 1965; Opechowski, 1986) for three-dimensional magnetic space groups. The specification was made in conjunction with Volume I of *International Tables for X-ray Crystallography* (1969) (abbreviated here as *ITXC* I). One finds in *ITXC* I, for each group type $\mathcal{F}$, a specification of the coordinate system used, and, in terms of that coordinate system, a specification of the subgroup of translations $\mathcal{T}$ of the representative space group of that group type, and also indirectly a specification of a set of coset representatives of $\mathcal{T}$ of that representative group of group type $\mathcal{F}$. These coset representatives are uniquely determined from the coordinate triplets of the explicitly printed general position of the space group. The symbol $\mathcal{F}$ for the space group is taken to be the space-group symbol at the top of the page listing these coordinate triplets. The symbol for a group type $\mathcal{F}1'$ is that of the group type $\mathcal{F}$ followed by $1'$, and the coset representatives of the representative group of the group type $\mathcal{F}1'$ consist of the set of coset representatives of $\mathcal{F}$ and this set multiplied by $1'$.

Example

In *ITXC* I, on the page for $\mathcal{F} = P2/m$ one finds the following coordinate triplets of the general position:

$$x, y, z; \quad x, y, \overline{z}; \quad \overline{x}, \overline{y}, z; \quad \overline{x}, \overline{y}, \overline{z}$$

determining the coset representative of the representative group $P2/m$:

$$\{1|0\}; \quad \{m_{001}|0\}; \quad \{2_{001}|0\}; \quad \{\overline{1}|0\}.$$

The coset representatives of the representative group $P2/m1'$ are then:

$$\begin{array}{llll} \{1|0\}; & \{m_{001}|0\}; & \{2_{001}|0\}; & \{\overline{1}|0\} \\ \{1|0\}'; & \{m_{001}|0\}'; & \{2_{001}|0\}'; & \{\overline{1}|0\}'. \end{array}$$

ITXC I has been replaced by *IT* A. Ones finds that, for some space groups, the set of coordinate triplets of the general positions explicitly printed in *IT* A differs from that explicitly printed in *ITXC* I. As a consequence, if one attempts to interpret the Opechowski–Guccione symbols (OG symbols) for magnetic groups using *IT* A, one will, in many cases misinterpret the meaning of the symbol (Litvin, 1997, 1998). [It was suggested in these two papers that the original set of OG symbols should be modified so one could correctly interpret them using *IT* A instead of *ITXC* I. Adopting this ill-advised suggestion would have required in the future a new modification of the OG symbols whenever changes were made to the choices of coordinate triplets of the general position in *IT* A. Consequently, the meaning of the original OG symbols was specified by Litvin (2001) by explicitly giving the coset representatives of the representative groups of each three-dimensional magnetic space group.]

Magnetic groups $\mathcal{M}_T$

The symbol for a magnetic group type $\mathcal{M}_T = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and its representative group is based on the symbol for the group type $\mathcal{F}$. $\mathcal{D}$ is an equi-translational subgroup of $\mathcal{F}$, *i.e.* the translational subgroup $\mathcal{T}^{\mathcal{M}_T}$ of the magnetic group $\mathcal{M}_T$ is $\mathcal{T}$, the translational subgroup of $\mathcal{F}$. The translational part of the group type symbol of an $\mathcal{M}_T$ group is then the same as that of the group type $\mathcal{F}$. A number or letter in the remaining part of the symbol of $\mathcal{F}$ appears unchanged in the symbol for $\mathcal{M}_T$ if it is associated with a coset representative of the representative group $\mathcal{F}$ that is also an element contained in the subgroup $\mathcal{D}$ of $\mathcal{F}$. If not in $\mathcal{D}$, *i.e.* if in $\mathcal{F} - \mathcal{D}$, the number or letter appears in the symbol for $\mathcal{M}_T$ with a prime to denote that the element in $\mathcal{M}_T$ is coupled with $1'$.

Example

The orthorhombic space-group type $\mathcal{F} = Pca2_1$ has the magnetic space-group type number 29.1.198. The representative group is defined by a orthorhombic translational subgroup $\mathcal{T}$ denoted by the letter P in $Pca2_1$ and the standard set of coset representatives

$$\{1|0\} \quad \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\} \quad \{m_{010}|\tfrac{1}{2}, 0, 0\} \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

The magnetic space-group type 29.5.202 is a group $\mathcal{M}_T$ whose symbol is $Pc'a'2_1$. In this case we have $Pc'a'2_1 = P2_1 \cup (Pca2_1 - P2_1)1'$, *i.e.* $\mathcal{F} = Pca2_1$ and $\mathcal{D} = P2_1$. The symbol '2_1' in the symbol for $\mathcal{F} = Pca2_1$ refers to the coset representative $\{2_{001}|0, 0, \frac{1}{2}\}$, an element in $\mathcal{D} = P2_1$. Consequently, the symbol '2_1' appears unprimed in the symbol for $\mathcal{M}_T$ ($Pc'a'2_1$) and the coset representative $\{2_{001}|0, 0, \frac{1}{2}\}$ appears as an unprimed coset representative in the standard set of coset representatives of $\mathcal{M}_T$. The symbols 'c' and 'a' in $\mathcal{F} = Pca2_1$ refer to the coset representatives $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, 0\}$, respectively, neither of which are contained in $\mathcal{D}$. Consequently, both symbols appear primed in the symbol $Pc'a'2_1$ for $\mathcal{M}_T$ and the coset representatives $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, 0\}$ appear as primed coset representatives in the standard set of coset representatives of $\mathcal{M}_T$. The representative magnetic space group $Pc'a'2_1$ then has the orthorhombic translational subgroup $\mathcal{T}$ denoted by the letter P and the standard set of coset representatives

$$\{1|0\} \quad \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}' \quad \{m_{010}|\tfrac{1}{2}, 0, 0\}' \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

Magnetic groups $\mathcal{M}_R$

The symbol for a group type $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and its representative group is also based on the symbol for the group $\mathcal{F}$. [This is in contradistinction to the BNS symbols of $\mathcal{M}_R$ groups (Belov *et al.*, 1957), where the symbol for an $\mathcal{M}_R$ group type is based on the symbol for the group $\mathcal{D}$, see Section 3.6.4.] As

this is an equi-class magnetic group, half the translations of $\mathcal{F}$ are now coupled with $1'$ in $\mathcal{M}_R$ and half the translations remain unprimed in $\mathcal{M}_R$. The unprimed translations constitute the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$. We can then write the coset decomposition of the translational subgroup $\mathcal{T}$ of $\mathcal{F}$ with respect to the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$ as

$$\mathcal{T} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha \mathcal{T}^{\mathcal{D}},$$

where t_α denotes a chosen coset representative, a translation of $\mathcal{F}$ which appears primed (coupled with $1'$) in $\mathcal{M}_R$. The translational subgroup $\mathcal{T}^{\mathcal{M}_R}$ of $\mathcal{M}_R$ can then be written as

$$\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}' \mathcal{T}^{\mathcal{D}}.$$

Symbols for the translational groups $\mathcal{T}$, the translational subgroups $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{T}$, the translational groups $\mathcal{T}^{\mathcal{M}_R}$ of $\mathcal{M}_R$ and the choice of the translations t_α are given in Fig. 1 of Litvin (2013).

The symbol for a magnetic group type $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$ and its representative group is based on the symbol of the group type $\mathcal{F}$, and is also a symbol for the subgroup $\mathcal{D}$ of unprimed elements: the translational part of the symbol of $\mathcal{F}$ is replaced by the symbol for the translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$. If a coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ of $\mathcal{T}$ in $\mathcal{F}$ appears as the coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R}) + \boldsymbol{t}_\alpha\}$ of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$, then the number or letter corresponding to $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ in the symbol for $\mathcal{F}$ is primed. If $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ appears unchanged as a coset representative of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$, then the number or letter corresponding to $\{\boldsymbol{R}|\boldsymbol{\tau}(\boldsymbol{R})\}$ in the symbol for $\mathcal{F}$ is unchanged (Opechowski & Litvin, 1977). The resulting symbol is a symbol for $\mathcal{D}$ based on the symbol for $\mathcal{F}$ and is also a symbol for the magnetic group $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$: the symbol specifies not only $\mathcal{D}$ but also $\mathcal{F}$; by deleting the subindex on the translational part of the symbol and the primes on the rotational part, one obtains the symbol specifying $\mathcal{F}$. Having specified $\mathcal{D}$ and $\mathcal{F}$, one has specified the group $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$.

Example

Consider again the group 29.1.198, $\mathcal{F} = Pca2_1$, where

$$\mathcal{F} = \{1|0\}\mathcal{T} \cup \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}\mathcal{T} \cup \{m_{010}|\tfrac{1}{2}, 0, 0\}\mathcal{T} \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}.$$

The symbol for the $\mathcal{M}_R = \mathcal{F}(\mathcal{D})$ group type 29.7.204 is $P_{2b}c'a'2_1$ and is based on the symbol for $\mathcal{F} = Pca2_1$. The translational subgroup $\mathcal{T}^{\mathcal{D}}$ of $\mathcal{D}$ is given by the symbol P_{2b} where t_α = $\{1|0, 1, 0\}$, *i.e.* $\mathcal{T}^{\mathcal{D}}$ is generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 2, 0\}$ and $\{1|0, 0, 1\}$ of $\mathcal{T}$, and the translational subgroup $\mathcal{T}^{\mathcal{M}_R}$ of $P_{2b}c'a'2_1$ is given by $\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}'\mathcal{T}^{\mathcal{D}}$. The two primed symbols c' and a' in $P_{2b}c'a'2_1$ refer to the fact that the two coset representatives $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 0, 0\}$ that appear in the set of standard coset representatives of $\mathcal{T}$ in $\mathcal{F}$ appear as the coset representatives $\{m_{100}|\frac{1}{2}, 1, \frac{1}{2}\}$ and $\{m_{010}|\frac{1}{2}, 1, 0\}$ in the set of standard coset representatives of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$. As the symbol 2_1 in $P_{2b}c'a'2_1$ is not primed, the coset representative $\{2_{001}|0, 0, \frac{1}{2}\}$ of $\mathcal{T}$ in $\mathcal{F}$ remains unchanged as a coset representative of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$. We have then the subgroup

$$\mathcal{D} = \{1|0\}\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{m_{010}|\tfrac{1}{2}, 1, 0\}\mathcal{T}^{\mathcal{D}} \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}}.$$

We note that these same coset representatives of $\mathcal{T}^{\mathcal{D}}$ in $\mathcal{D}$ are also the coset representatives of the standard set of coset representatives of $\mathcal{T}^{\mathcal{M}_R}$ in $\mathcal{M}_R$.

$$\mathcal{M}_R = \{1|0\}\mathcal{T}^{\mathcal{M}_R} \cup \{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{M}_R} \cup \{m_{010}|\tfrac{1}{2}, 1, 0\}\mathcal{T}^{\mathcal{M}_R} \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{M}_R}$$

and the standard set of coset representatives of $P_{2b}c'a'2_1$ listed in the tables is the same set of coset representatives:

$$\{1|0\} \quad \{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\} \quad \{m_{010}|\tfrac{1}{2}, 1, 0\} \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

Since $\mathcal{T}^{\mathcal{M}_R} = \mathcal{T}^{\mathcal{D}} \cup t_\alpha{}'\mathcal{T}^{\mathcal{D}}$, it follows that $\mathcal{M}_R = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$ and

$$\mathcal{M}_R = \{1|0\}\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2}, 1, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{m_{010}|\tfrac{1}{2}, 1, 0\}\mathcal{T}^{\mathcal{D}} \cup \{2_{001}|0, 0, \tfrac{1}{2}\}\mathcal{T}^{\mathcal{D}} \cup \{1|0, 1, 0\}'\mathcal{T}^{\mathcal{D}} \cup \{m_{100}|\tfrac{1}{2}, 0, \tfrac{1}{2}\}'\mathcal{T}^{\mathcal{D}} \cup \{m_{010}|\tfrac{1}{2}, 0, 0\}'\mathcal{T}^{\mathcal{D}} \cup \{2_{001}|0, 1, \tfrac{1}{2}\}'\mathcal{T}^{\mathcal{D}}.$$

Consequently, a primed number or letter in the symbol for $\mathcal{M}_R$ (which is also a symbol for $\mathcal{D}$) denotes that the corresponding coset representative appears in $\mathcal{D}$ coupled with t_α and primed in $(\mathcal{F} - \mathcal{D})1'$, *e.g.* a' in $P_{2b}c'a'2_1$ denotes that the coset $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}$ appears as $\{m_{100}|\frac{1}{2}, 1, \frac{1}{2}\}$ in $\mathcal{D}$ and as $\{m_{100}|\frac{1}{2}, 0, \frac{1}{2}\}'$ in $(\mathcal{F} - \mathcal{D})1'$. An unprimed number or letter in the symbol for $\mathcal{M}_R$ (which is also a symbol for $\mathcal{D}$) denotes that the corresponding element appears unchanged in $\mathcal{D}$ and coupled with t_α and primed in $(\mathcal{F} - \mathcal{D})1'$, *e.g.* the symbol 2_1 in $P_{2b}c'a'2_1$ denotes that $\{2_{001}|0, 0, \frac{1}{2}\}$ is in $\mathcal{D}$ and $\{2_{001}|1, 0, \frac{1}{2}\}'$ is in $(\mathcal{F} - \mathcal{D})1'$.

For two-dimensional magnetic space groups with square and hexagonal lattices, three-dimensional magnetic space groups with tetragonal, hexagonal, rhombohedral and cubic lattices, and magnetic layer and rod groups with tetragonal, trigonal or hexagonal lattices, each letter or number in the group type symbol may represent not a single symmetry direction but a set of symmetry directions, see Table 1.3 in Litvin (2013), Table 2.1.3.1 in the present volume and Table 1.2.4.1 in *IT* E. Stokes & Campbell (2009) have pointed out that this can lead to not being able to determine the standard set of coset representatives in $\mathcal{M}_R$ groups from the Opechowski–Guccione magnetic group symbol. Consequently, we introduce the convention that in determining the standard set of coset representatives, each letter or number in the group type symbol in these groups refers to the first symmetry direction of each set of symmetry directions listed in the aforementioned tables.

Example

The standard set of coset representatives of 94.1.786 $P4_22_12$ is

$$\begin{array}{llll} \{1|0\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{001}|0\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\} \\ \{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{010}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{110}|0\}; & \{2_{1\bar{1}0}|0\}. \end{array}$$

For the three-dimensional magnetic group 94.7.792 $P_{2c}4'_22'_12$, the standard set of coset representatives is

$$\begin{array}{llll} \{1|0\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}\}; & \{2_{001}|0, 0, 1\}; & \{4_{001}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\} \\ \{2_{100}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{3}{2}\}; & \{2_{010}|\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}\}; & \{2_{110}|0, 0, 1\}; & \{2_{1\bar{1}0}|0\}. \end{array}$$

The secondary position in the Hermann–Mauguin symbol $P_{2c}4'_22'_12$ denotes the set of symmetry directions {[100], [010]}. With this convention, the primed symbol $2'_1$ denotes that the corresponding coset representative $\{2_{100}|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$ of $P4_22_12$ appears in the coset representatives of $P_{2c}4'_22'_12$ coupled with the translation t_α = $\{1|0, 0, 1\}$. The third position in the Hermann–Mauguin symbol $P_{2c}4'_22'_12$ denotes the set of symmetry directions $\{[1\bar{1}0], [110]\}$. The unprimed symbol 2 denotes that the coset representative $\{2_{1\bar{1}0}|0\}$ of $P4_22_12$ appears unchanged in the coset representatives of $P_{2c}4'_22'_12$.

The impact of this convention is that nine Opechowski–Guccione symbols of three-dimensional magnetic space groups need to be changed:

	Old symbol	New symbol
93.6.781	$P_{2c}4_222$	$P_{2c}4_222'$
93.8.783	P_I4_222	P_I4_222'
93.9.784	$P_{2c}4_2'22'$	$P_{2c}4_2'22$
153.4.1270	$P_{2c}3_112$	$P_{2c}3_112'$
154.4.1274	$P_{2c}3_121$	$P_{2c}3_12'1$
180.6.1401	$P_{2c}6_222$	$P_{2c}6_222'$
180.7.1402	$P_{2c}6_2'22'$	$P_{2c}6_2'22$
181.6.1408	$P_{2c}6_422$	$P_{2c}6_422'$
181.7.1409	$P_{2c}6_4'2'2$	$P_{2c}6_4'2'2'$

To have all $\mathcal{M}_R$ group symbols represent subgroups $\mathcal{D}$, six symbols for three-dimensional magnetic space groups were based (Opechowski & Guccione, 1965) on the symbol of the subgroup $\mathcal{D}$ instead of the symbol for $\mathcal{F}$. These are the groups 144.3.1236 $P_{2c}3_2$, 145.3.1239 $P_{2c}3_1$, 151.4.1262 $P_{2c}3_212$, 152.4.1266 $P_{2c}3_221$, 153.4.1270 $P_{2c}3_112$ and 154.4.1274 $P_{2c}3_121$. Additional groups are the rod groups 43.3.231 $\not{P}_{2c}3_2$, 44.3.234 $\not{P}_{2c}3_1$, 47.4.246 $\not{P}_{2c}3_212$ and 48.4.250 $\not{P}_{2c}3_112$.

3.6.2.2.5. Symbol of the subgroup $\mathcal{D}$ of index 2 of $\mathcal{F}(\mathcal{D})$

For magnetic group types $\mathcal{F}(\mathcal{D})$, the magnetic group type symbol of the subgroup $\mathcal{D}$ is given in the third column of the survey of magnetic groups, see *e.g.* Table 3.6.2.2. If $\mathcal{F}(\mathcal{D})$ is a group $\mathcal{M}_T$, then the subgroup $\mathcal{D}$ is defined by the translational group of $\mathcal{F}(\mathcal{D})$ and the unprimed coset representatives of $\mathcal{F}(\mathcal{D})$.

Example

Consider the three-dimensional magnetic space-group type 16.3.101 $P2'2'2$. The representative group $P2'2'2$ is defined by the translational subgroup $\mathcal{T}$ denoted by the letter P generated by the translations

$$\{1|1, 0, 0)\} \quad \{1|0, 1, 0\} \quad \{1|0, 0, 1\}$$

and the standard set of coset representatives

$$\{1|0\} \quad \{2_{100}|0\}' \quad \{2_{010}|0\}' \quad \{2_{001}|0\}.$$

The subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D}) = P2'2'2$ is defined by the translational group $\mathcal{T}$ denoted by the letter P and the cosets $\{1|0\}$ and $\{2_{001}|0\}$, and is a group of type $P2$.

If $\mathcal{F}(\mathcal{D})$ is a group $\mathcal{M}_R$, then the subgroup $\mathcal{D}$ is defined by the non-primed translational group of $\mathcal{F}(\mathcal{D})$ and all the cosets of the standard set of coset representatives of the group $\mathcal{F}(\mathcal{D})$.

Example

Consider the three-dimensional magnetic space-group type 16.4.102 $P_{2a}222$. The representative group $P_{2a}222$ is defined by the translational group $\mathcal{T}$ denoted by the symbol P_{2a} generated by the translations

$$\{1|1, 0, 0\}' \quad \{1|0, 1, 0\} \quad \{1|0, 0, 1\}$$

and the standard set of coset representatives

$$\{1|0\} \quad \{2_{100}|0\} \quad \{2_{010}|0\} \quad \{2_{001}|0\}.$$

The subgroup $\mathcal{D}$ of index 2 of the representative group $\mathcal{F}(\mathcal{D}) = P_{2a}222$ is defined by the translational subgroup $\mathcal{T}$ denoted by the symbol P_{2a}, *i.e.* the translations generated by

$$\{1|2, 0, 0\} \quad \{1|0, 1, 0\} \quad \{1|0, 0, 1\}$$

and the standard set of cosets of $P_{2a}222$. The group $\mathcal{D}$ is a group of type $P222$.

While the group type symbol of $\mathcal{D}$ is given, the coset representatives of the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ derived from the standard set of coset representatives of $\mathcal{F}(\mathcal{D})$ may not be identical with the standard set of coset representatives of the representative group of type $\mathcal{D}$ found in the survey of magnetic group types. Consequently, to show the relationship between this subgroup $\mathcal{D}$ and the listed representative group of groups of type $\mathcal{D}$ additional information is provided: a new coordinate system is defined in which the coset representatives of this subgroup $\mathcal{D}$ are identical with the standard set of coset representatives listed for the representative group of groups of type $\mathcal{D}$: Let (O; **a**, **b**, **c**) be the coordinate system in which the group $\mathcal{F}(\mathcal{D})$ is defined. O is the origin of the coordinate system, and **a**, **b** and **c** are the basis vectors of the coordinate system. **a**, **b** and **c** represent a set of basis vectors of a primitive cell for primitive lattices and of a conventional cell for centred lattices. A second coordinate system, defined by (O + **p**; **a**′, **b**′, **c**′), is given in which the coset representatives of this subgroup $\mathcal{D}$ are identical with the standard set of coset representatives listed for the representative group of groups of type $\mathcal{D}$. O + **p** is referred to as the *location* of the subgroup $\mathcal{D}$ in the coordinate system of the group $\mathcal{F}(\mathcal{D})$ (Kopský, 2011). The origin is first translated from O to O + **p**. On translating the origin from O to O + **p**, a coset representative $\{\boldsymbol{R}|\boldsymbol{\tau}\}$ becomes $\{\boldsymbol{R}|\boldsymbol{\tau} + \boldsymbol{Rp} - \boldsymbol{p}\}$ (Litvin, 2005, 2008*b*; see also Section 1.5.2.3). This is followed by changing the basis vectors **a**, **b** and **c** to **a**′, **b**′ and **c**′, respectively. The basis vectors **a**′, **b**′, **c**′ define the conventional unit cell of the non-primed subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ in the coordinate system (O; **a**, **b**, **c**) in which $\mathcal{F}(\mathcal{D})$ is defined. (O + **p**; **a**′, **b**′, **c**′) is given immediately following the group type symbol for the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$. [In Litvin (2013), for typographical simplicity, the symbols 'O +' are omitted.]

Example

For the three-dimensional magnetic space-group type 10.4.52, $\mathcal{F}(\mathcal{D}) = P2/m'$, one finds in Litvin (2013)[2]

Serial No.	Symbol	Non-primed subgroup of index 2	Standard set of coset representatives
10.4.52	$P2/m'$	$P2$ (0, 0, 0; **a**, **b**, **c**)	$\{1\|0\}$ $\{2_{010}\|0\}$ $\{1\|0\}'$ $\{m_{010}\|0\}'$

The translational subgroup of the subgroup $\mathcal{D}$ = $P2$ of $\mathcal{F}(\mathcal{D}) = P2/m'$ is generated by the translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 1\}$ and the coset representatives of this group are $\{1|0\}$ and $\{2_{010}|0\}$, the unprimed coset representatives on the right. This subgroup $\mathcal{D}$ is of type $P2$. In Litvin (2013), listed for the group type 3.1.8, $P2$, one finds the identical two coset representatives. Consequently, there is no change in the coordinate system, *i.e.* **p** = (0, 0, 0) and **a**′ = **a**, **b**′ = **b** and **c**′ = **c**. In the coordinate system of the magnetic group $P2/m'$, the coset representatives of its subgroup $\mathcal{D} = P2$ are identical with the standard set of coset representatives of the group type $P2$.

[2] In Litvin (2013) the terminology 'non-magnetic' is used in place of 'non-primed' in the column headings in these tables.

Example

For the three-dimensional magnetic space-group type 16.7.105, $\mathcal{F}(\mathcal{D}) = P_{2c}22'2'$ one has

Serial No.	Symbol	Non-primed subgroup of index 2	Standard set of coset representatives
16.7.105	$P_{2c}22'2'$	$P222_1$ (0, 0, 0; **a**, **b**, 2**c**)	{1|0} {2_{100}|0} {2_{010}|0, 0, 1} {2_{001}|0, 0, 1}

The translational subgroup of the subgroup $\mathcal{D} = P222_1$ of $\mathcal{F}(\mathcal{D}) = P_{2c}22'2'$ is generated by the translations {1|1, 0, 0}, {1|0, 1, 0} and {1|0, 0, 2}, and the coset representatives of this group are all those coset representatives on the right. This subgroup $\mathcal{D}$ is of type $P222_1$. Listed for the group type 17.1.106 $P222_1$, one finds a different set of coset representatives:

$$\{1|0\} \quad \{2_{100}|0\} \quad \{2_{010}|0, 0, \tfrac{1}{2}\} \quad \{2_{001}|0, 0, \tfrac{1}{2}\}.$$

Consequently, to show the relationship between this subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ and the listed representative group of the group type $P222_1$ we change the coordinate system in which $\mathcal{D}$ is defined to (0, 0, 0; **a**, **b**, 2**c**). In this new coordinate system the coset representatives of the subgroup $\mathcal{D}$ are identical with the coset representatives of the representative group of the group type $P222_1$.

Example

For the three-dimensional magnetic space-group type 18.4.116, $P2_12_1'2'$, one has

Serial No.	Symbol	Non-primed subgroup of index 2	Standard set of coset representatives
18.4.116	$P2_12_1'2'$	$P2_1$ (0, $\frac{1}{4}$, 0; **c**, **a**, **b**)	{1|0} {2_{100}|$\frac{1}{2}$, $\frac{1}{2}$, 0} {2_{010}|$\frac{1}{2}$, $\frac{1}{2}$, 0}′ {2_{001}|0}′

The translational subgroup of $\mathcal{D}$ is generated by the translations {1|1, 0, 0}, {1|0, 1, 0} and {1|0, 0, 1} and the coset representatives of this group are {1|0} and {2_{100}|$\frac{1}{2}$, $\frac{1}{2}$, 0}, the unprimed coset representatives on the right. The group $\mathcal{D}$ is of type $P2_1$. For the magnetic group type 4.1.15 $P2_1$ one finds a different set of coset representatives: {1|0} and {2_{010}|0, $\frac{1}{2}$, 0}. Consequently, to show the relationship between the subgroup $\mathcal{D}$ of $\mathcal{F}(\mathcal{D})$ and the listed representative group of the group type $P2_1$, we change the coordinate system in which the subgroup $\mathcal{D}$ is defined to (0, $\frac{1}{4}$, 0; **c**, **a**, **b**). The origin is first translated from O to $O + \mathbf{p}$, where $\mathbf{p} = (0, \frac{1}{4}, 0)$, and then a new set of basis vectors, $\mathbf{a}' = \mathbf{c}$, $\mathbf{b}' = \mathbf{a}$ and $\mathbf{c}' = \mathbf{b}$, is defined. In this new coordinate system the coset representatives of the subgroup $\mathcal{D}$ are identical with the standard set of coset representatives of the representative group of the group type $P2_1$.

3.6.3. Tables of properties of magnetic groups

In this section we present a guide to the tables of properties of the two- and three-dimensional magnetic subperiodic groups and the one-, two- and three-dimensional magnetic space groups given by Litvin (2013). The format and content of these magnetic group tables are similar to the format and content of the space-group tables in the present volume, the subperiodic group tables in *IT* E, and previous compilations of magnetic subperiodic groups (Litvin, 2005) and magnetic space groups (Litvin, 2008*b*). An example of one these tables is given in Fig. 3.6.3.1. The tables of properties of magnetic groups contain:

First page:

(1) Lattice diagram
(2) Headline
(3) Diagrams of symmetry elements and of the general positions
(4) Origin
(5) Asymmetric unit
(6) Symmetry operations

Subsequent pages:

(7) Abbreviated headline
(8) Generators selected
(9) General and special positions with spins (magnetic moments)
(10) Symmetry of special projections

Tabulations of properties of three-dimensional magnetic space groups can also be found in Koptsik (1968) (note that the general-position diagrams are of 'black and white' objects, not spins). Neutron-diffraction extinctions can be found in the work of Ozerov (1969*a*,*b*) and on the Bilbao Crystallographic Server, http://www.cryst.ehu.es (Aroyo *et al.*, 2006). General positions and Wyckoff positions of the three-dimensional magnetic space groups can also be found on the Bilbao Crystallographic Server.

3.6.3.1. Lattice diagram

For each three-dimensional magnetic space group, a three-dimensional lattice diagram is given in the upper left-hand corner of the first page of the tables of properties of that group. (For all other magnetic groups, the corresponding lattice diagram is given within the symmetry diagram, see Section 3.6.3.3 below.) This lattice diagram depicts the coordinate system used, the conventional unit cell of the space group $\mathcal{F}$, the magnetic space group's magnetic superfamily type and the generators of the translational subgroup of the magnetic space group. In Fig. 3.6.3.2 we show lattice diagrams for two orthorhombic magnetic space groups: (*a*) $Pmc2_1$ and (*b*) $P_{2b}m'c'2_1$. The generating lattice vectors are colour coded. Those coloured black are not coupled with time inversion, while those coloured red are coupled with time inversion. In the group $Pmc2_1$, a magnetic group of the type $\mathcal{F}$, the lattice is an orthorhombic P lattice, see Fig. 3.6.3.2(*a*), and no generating translation is coupled with time inversion. In the second group, $P_{2b}m'c'2_1$, a magnetic group of type $\mathcal{M}_R$, the lattice is an orthorhombic P_{2b} lattice, see Fig. 3.6.3.2(*b*), and the generating lattice vector in the y direction is coupled with time inversion.

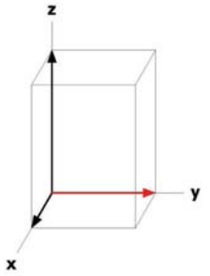
3.6.3.2. Heading

Each table begins with a headline consisting of two lines with five entries, for example

$P4/m'mm$	$4/m'mm$	Tetragonal
123.3.1001	$P4/m'2'/m2'/m$	

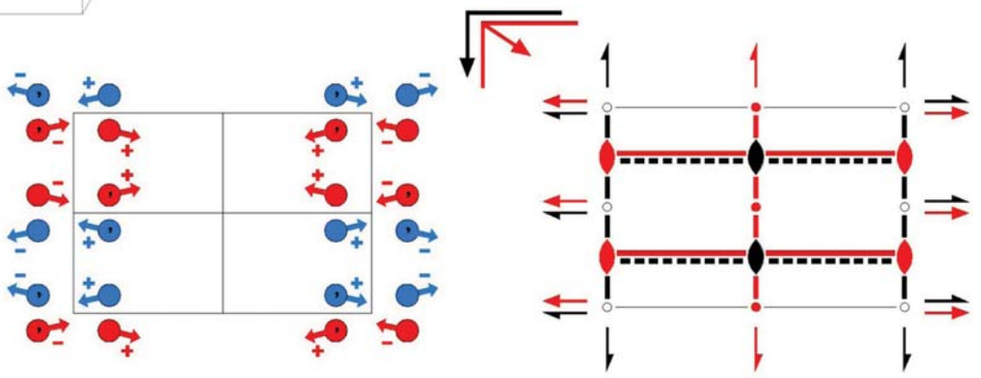
For three-dimensional magnetic space groups, this headline is to the right of the lattice diagram. On the upper line, starting on the left, are three entries:

(1) The *short international* (Hermann–Mauguin) *symbol* of the magnetic space group. Each symbol has two meanings: The first is that of the Hermann–Mauguin symbol of a magnetic space-group type. The second is that of a specific magnetic space group, the representative magnetic space group (see Section 3.6.2.2), which belongs to this magnetic space-group



P_{2b}m'ma **mmm1'** Orthorhombic

51.13.399 **$P_{2b}2_1$/m'2'/m2'/a**



Origin at center (2'/m) at $2_12/ma$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

Symmetry Operations

For (0,0,0) + set

(1) 1	(2) 2' ¼,0,z	(3) 2' 0,y,0	(4) 2 (½,0,0) x,0,0
{1 | 0}	{2_{001} | ½,0,0}'	{2_{010} | 0}'	{2_{100} | ½,0,0}
(5) $\bar{1}$'	(6) a (½,0,0) x,y,0	(7) m x,0,z	(8) m' ¼,y,z
{$\bar{1}$ | 0}'	{m_{001} | ½,0,0}	{m_{010} | 0}	{m_{100} | ½,0,0}'

For (0,1,0)' + set

(2) t' (0,1,0)'	(2) 2 ¼,½,z	(3) 2 (0,1,0) 0,y,0	(4) 2' (½,0,0) x,½,0
{1 | 0,1,0}'	{2_{001} | ½,1,0}	{2_{010} | 0,1,0}	{2_{100} | ½,1,0}'
(5) $\bar{1}$ (0, ½,0)	(6) n' (½,1,0) x,y,0	(7) m' x,½,z	(8) b (0,1,0) ¼,y,z
{$\bar{1}$ | 0,1,0}	{m_{001} | ½,1,0}'	{m_{010} | 0,1,0}'	{m_{100} | ½,1,0}

Figure 3.6.3.1
Table of properties of the three-dimensional magnetic space group 51.13.399 $P_{2b}m'ma$.

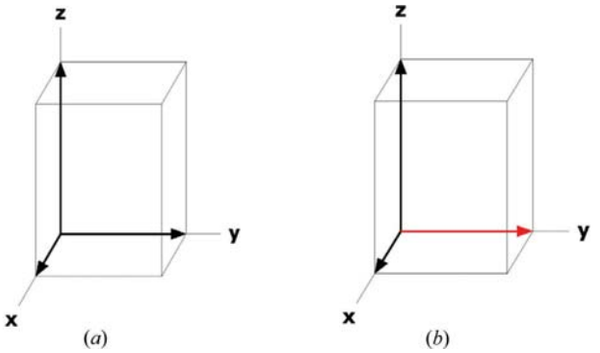


Figure 3.6.3.2
Lattice diagrams of (*a*) the three-dimensional magnetic space group 26.1.168 $\mathcal{F} = Pmc2_1$ and (*b*) the three-dimensional magnetic space group 26.10.177 $\mathcal{M}_R = P_{2b}m'c'2_1 = \mathcal{F}(\mathcal{D}) = Pmc2_1(Pca2_1)$.

type. Given a coordinate system, this group is defined by the list of symmetry operations (see Section 3.6.3.6) given on the page with this Hermann–Mauguin symbol in the heading, or by the given list of general positions and magnetic moments (see Section 3.6.3.9).

(2) The *short international* (Hermann–Mauguin) *point group symbol* for the geometric crystal class to which the magnetic space group belongs.

(3) The crystal system or crystal system/Bravais system classification to which the magnetic space group belongs.

The second line has two additional entries:

(4) The three-part numerical serial index of the magnetic group (see Section 3.6.2.2.1).

(5) The *full international (Hermann–Mauguin) symbol* of the magnetic space group.

Continued 51.13.399 **P_{2b}m'ma**

Generators selected (1); t (1,0,0); t (0,1,0)'; t (0,0,1); (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site Symmetry	Coordinates (0,0,0) +	(0,1,0)' +		
16 l 1	(1) x,y,z [u,v,w]	(2) $\bar{x}$+½,$\bar{y}$,z [u,v,$\bar{w}$]	(3) $\bar{x}$,y,$\bar{z}$ [u,$\bar{v}$,w]	(4) x+½,$\bar{y}$,$\bar{z}$ [u,$\bar{v}$,$\bar{w}$]
	(5) $\bar{x}$,$\bar{y}$,$\bar{z}$ [$\bar{u}$,$\bar{v}$,$\bar{w}$]	(6) x+ ½,y,$\bar{z}$ [$\bar{u}$,$\bar{v}$,w]	(7) x,$\bar{y}$,z [$\bar{u}$,v,$\bar{w}$]	(8) $\bar{x}$+½,y,z [$\bar{u}$,v,w]
8 k m'..	¼,y,z [0,v,w]	¼,$\bar{y}$,z [0,v,$\bar{w}$]	¾,y,$\bar{z}$ [0,$\bar{v}$,w]	¾,$\bar{y}$,$\bar{z}$ [0,$\bar{v}$,$\bar{w}$]
8 j .m'.	x,½,z [u,0,w]	$\bar{x}$ + ½,½,z [$\bar{u}$,0,w]	$\bar{x}$,½,$\bar{z}$ [u,0,w]	x+ ½,½,$\bar{z}$ [$\bar{u}$,0,w]
8 i .m.	x,0,z [0,v,0]	$\bar{x}$ + ½,½,z [0,v,0]	$\bar{x}$,0,$\bar{z}$ [0,$\bar{v}$,0]	x+ ½,0,$\bar{z}$ [0,$\bar{v}$,0]
8 h .2'.	0,y,½ [u,0,w]	½,$\bar{y}$,½ [u,0,$\bar{w}$]	0,$\bar{y}$,½ [$\bar{u}$,0,$\bar{w}$]	½,y,½ [$\bar{u}$,0,w]
8 g .2'.	0,y,0 [u,0,w]	½,$\bar{y}$,0 [u,0,$\bar{w}$]	0,$\bar{y}$,0 [$\bar{u}$,0,$\bar{w}$]	½,y,0 [$\bar{u}$,0,w]
4 f m'm'2	¼,½,z [0,0,w]	¾,½,$\bar{z}$ [0,0,w]		
4 e m'm2'	¼,0,z [0,v,0]	¾,0,$\bar{z}$ [0,$\bar{v}$,0]		
4 d .2'/m'.	0,½,½ [u,0,w]	½,½,½ [$\bar{u}$,0,w]		
4 c .2'/m.	0,0,½ [0,0,0]	½,0,½ [0,0,0]		
4 b .2'/m'.	0,½,0 [u,0,w]	½,½,0 [$\bar{u}$,0,w]		
4 a .2'/m.	0,0,0 [0,0,0]	½,0,0 [0,0,0]		

Symmetry of Special Projections

Along [0,0,1] **p_{c*}2mm**	Along [1,0,0] **p_{2a*}2mm**	Along [0,1,0] **p2mg1'**
a* = **-a**/2 **b*** = **b**	**a*** = **b** **b*** = **c**	**a*** = **-a** **b*** = **c**
Origin at 0,0,z	Origin at x,0,0	Origin at 0,y,0

Figure 3.6.3.1
Table of properties of the three-dimensional magnetic space group 51.13.399 $P_{2b}m'ma$ continued.

3.6.3.3. Diagrams of symmetry elements and of the general positions

There are two types of diagrams: symmetry diagrams and general-position diagrams. The symmetry diagrams show (1) the relative locations and orientations of the symmetry elements and (2) the absolute locations and orientations of these symmetry elements in a given coordinate system. The general-position diagrams show, in that coordinate system, the arrangement of a set of symmetry-equivalent general points and the relative orientations of magnetic moments on this set of points. Figs. 3.6.3.3 and 3.6.3.4 show the symmetry diagram and general-position diagram, respectively, of the three-dimensional magnetic space group $P4_12'2'$.

All diagrams of three-dimensional magnetic space groups and three-dimensional subperiodic groups are orthogonal projections. The projection direction is along a basis vector of the conventional crystallographic coordinate system, see Table 1.1 of Litvin (2013). If the other two basis vectors are not parallel to the plane of the diagram, they are indicated by a subscript p, *e.g.* $\mathbf{a}_p$, $\mathbf{b}_p$ and $\mathbf{c}_p$. Schematic representations of the diagrams, showing their conventional coordinate systems, *i.e.* the origin O and basis vectors, are given in Table 2.1 of Litvin (2013). For two-dimensional magnetic space groups and magnetic frieze groups, the diagrams are in the plane defined by the group's conventional coordinate system.

The graphical symbols used in the symmetry diagrams are listed in Table 2.2 of Litvin (2013) and are an extension of those used in the present volume, *IT* E and Litvin (2008*b*). For symmetry planes and symmetry axes parallel to the plane of diagram, for rotation-inversions and for centres of symmetry, the 'heights' h along the projection direction above the plane of the

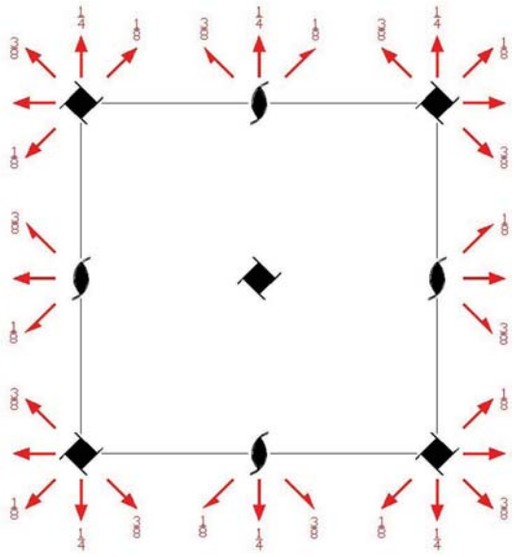


Figure 3.6.3.3
Symmetry diagram of $P4_12'2'$

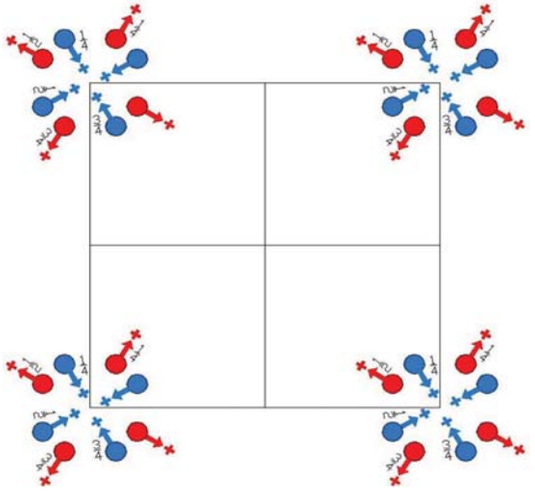


Figure 3.6.3.4
General-position diagram of $P4_12'2'$.

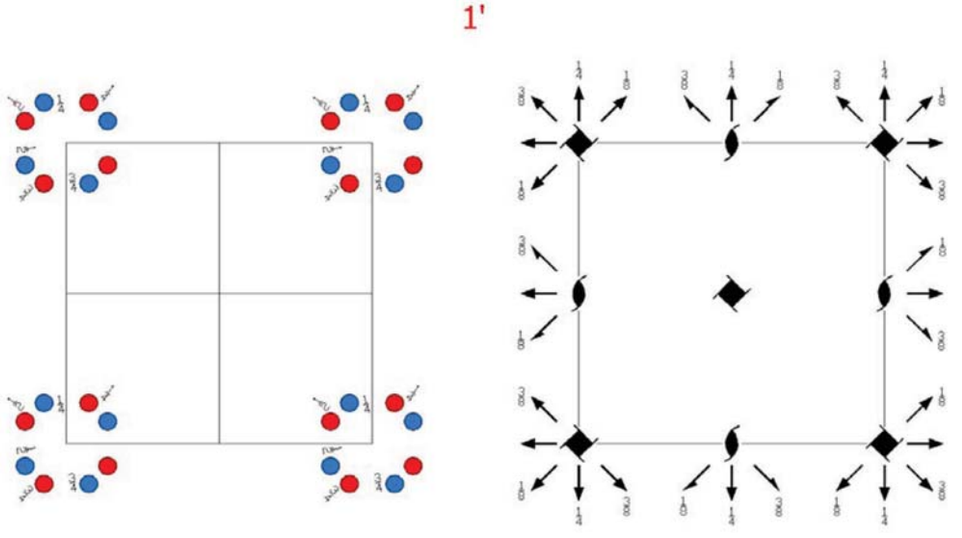


Figure 3.6.3.5
Diagrams of the magnetic space group $P4_1221'$.

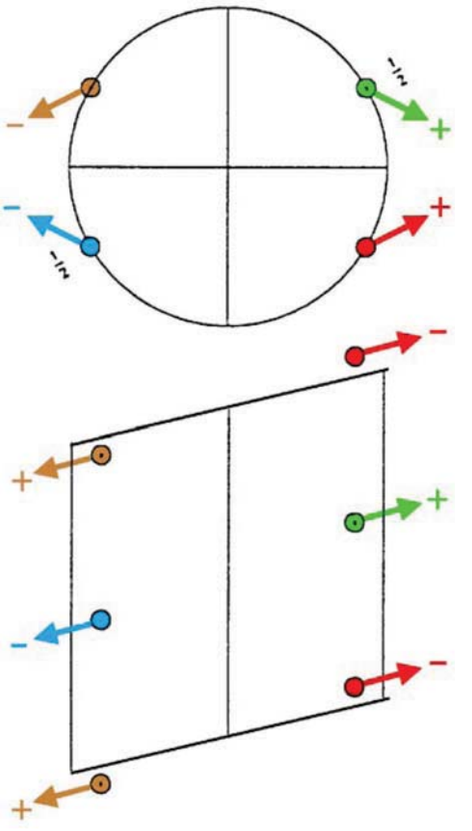


Figure 3.6.3.6
General-position diagram of rod group 2.3.29 $P2/c'11$. The positional colour coding is red for $x > 0$ and $z > 0$; blue for $x > 0$ and $z < 0$; green for $x < 0$ and $z > 0$; and brown for $x < 0$ and $z < 0$.

diagram are given. The heights are given as fractions of the shortest translation along the projection direction and, if different from zero, are printed next to the graphical symbol, see Fig. 3.6.3.3.

In the general-position diagrams, the general positions and corresponding magnetic moments are colour coded. Positions with a z component of $+z$ are shown as red circles and those with a z component of $-z$ are shown as blue circles. If the z component is either $h + z$ or $h - z$ with $h \neq 0$, then the height h is printed next to the general position, see Fig. 3.6.3.4. If two general positions have the same x component and y component, but one has a z component $+z$ and the other $-z$, the positions are shown as a circle with one half coloured red, the other half blue. The magnetic moments are colour coded to the general position to which they are associated, their direction in the plane of projection is given by an arrow in the direction of the projected magnetic moment. A + or − sign near the tip of the arrow indicates that the magnetic moment is inclined, respectively, above or below the plane of projection.

For magnetic space groups of the type $\mathcal{F}1'$, the symmetry diagram is that of the group $\mathcal{F}$. That each

symmetry element also appears coupled with time inversion is represented by a red 1′ printed between and above the general-position and symmetry diagrams. Because groups of this type contain the time-inversion symmetry, the magnetic moments are all identically zero, and no arrows appear in the general-position diagram. An example, the diagrams of the magnetic space group $P4_1221'$ are shown in Fig. 3.6.3.5. For triclinic, monoclinic/oblique, monoclinic/rectangular and orthorhombic rod groups, the colour coding of the general positions is extended according to the positive or negative values of the x and z components of the coordinates of the general position, see Fig. 3.6.3.6.

Table 3.6.3.1
Symmetry operations of magnetic space group 51.14.400 $P_{2b}mma'$

Symmetry operations			
	For (0, 0, 0)+ set		
(1) 1 {1|0}	(2) 2 1/4, 0, z $\{2_{001}\|1/2, 0, 0\}$	(3) 2′ 0, y, 0 $\{2_{010}\|0\}'$	(4) 2′ (1/2, 0, 0) x, 0, 0 $\{2_{100}\|1/2, 0, 0\}'$
(5) $\bar{1}'$ $\{\bar{1}\|0\}'$	(6) a' (1/2, 0, 0) x, y, 0 $\{m_{001}\|1/2, 0, 0\}'$	(7) m x, 0, z $\{m_{010}\|0\}$	(8) m 1/4, y, z $\{m_{100}\|1/2, 0, 0\}$
	For (0, 1, 0)′+ set		
(1) t' (0, 1, 0) $\{1\|0, 1, 0\}'$	(2) 2′ 1/4, 1/2, z $\{2_{001}\|1/2, 1, 0\}'$	(3) 2 (0, 1, 0) 0, y, 0 $\{2_{010}\|0, 1, 0\}$	(4) 2 (1/2, 0, 0) x, 1/2, 0 $\{2_{100}\|1/2, 1, 0\}$
(5) $\bar{1}$ 0, 1/2, 0 $\{\bar{1}\|0, 1, 0\}$	(6) n (1/2, 1, 0) x, y, 0 $\{m_{001}\|1/2, 1, 0\}$	(7) m' x, 1/2, z $\{m_{010}\|0, 1, 0\}'$	(8) b (0, 1, 0) 1/4, y, z $\{m_{100}\|1/2, 1, 0\}'$

VRML (Virtual Reality Modeling Language) general-position diagrams are available for the two- and three-dimensional magnetic subperiodic groups (Cordisco & Litvin, 2004), and for the one-, two- and non-cubic three-dimensional magnetic space groups (Burke *et al.*, 2006). These diagrams can be rotated and zoomed in on to aid in the visualization of the general-position diagrams, and include both the general positions of the atoms and the general orientations of the associated magnetic moments.

3.6.3.4. Origin

If the magnetic space group is centrosymmetric, then the inversion centre or a position of high site symmetry, as on the fourfold axis of tetragonal groups, is chosen as the origin. For noncentrosymmetric groups, the origin is at a point of highest site symmetry. If no site symmetry is higher than 1, the origin is placed on a screw axis, a glide plane or at the intersection of several such symmetries.

In the *Origin* line below the diagrams, the site symmetry of the origin is given. An additional symbol indicates all symmetry elements that pass through the origin. For example, for the magnetic space group $I4/mcm$, one finds '**Origin** at center (4/m) at $4/mc2_1/c$'. The site symmetry is 4/m and, in addition, two glide planes perpendicular to the y and z axes, and a screw axis parallel to the z axis, pass through the origin.

3.6.3.5. Asymmetric unit

An asymmetric unit is a simply connected smallest part of space which, by application of all symmetry operations of the magnetic group, exactly fills the whole space. For subperiodic groups, because the translational symmetry is of a lower dimension than that of the space, the asymmetric unit is infinite in size. The asymmetric unit for subperiodic groups is defined by setting the limits on the coordinates of points contained in the asymmetric unit. For example, the asymmetric unit for the magnetic layer group 32.3.199 $pm'2_1n'$ is

Asymmetric unit $0 < x < \frac{1}{2}$; $0 < y < 1$; $0 < z$

Since the translational symmetry of a magnetic space group is of the same dimension as that of the space, the asymmetric unit is a finite part of space. The asymmetric unit is defined, as above, by setting the limits on the coordinates of points contained in the asymmetric unit. For example, for the magnetic space group 140.3.1198 $I4/m'cm$ one has

Asymmetric unit $0 < x < \frac{1}{2}$; $0 < y < \frac{1}{2}$; $0 < z < \frac{1}{4}$; $y < \frac{1}{2} - x$

Drawings showing the boundary planes occurring in the tetragonal, trigonal and hexagonal systems, together with their algebraic equations, are given in Fig. 2.1.3.11. Drawings of asymmetric units for cubic groups have been published by Koch & Fischer (1974). The asymmetric units have complicated shapes in the trigonal, hexagonal and cubic crystal systems, and consequently are also specified by giving the vertices of the asymmetric unit. For example, for the magnetic space group 176.1.1374 $P6_3/m$ one finds

Asymmetric unit		$0 < x < 2/3$; $x < (1 + y)/2$;	$0 < y < 2/3$; $y < \min(1 - x, (1 + x)/2)$	$0 < z < 1/4$;	
Vertices	0, 0, 0	1/2, 0, 0	2/3, 1/3, 0	1/3, 2/3, 0	0, 1/2, 0
	0, 0, 1/4	1/2, 0, 1/4	2/3, 1/3, 1/4	1/3, 2/3, 1/4	0, 1/2, 1/4

Because the asymmetric unit is invariant under time inversion, all magnetic space groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{F}(\mathcal{D})$ of the magnetic superfamily of type $\mathcal{F}$ have identical asymmetric units, the asymmetric unit of the group $\mathcal{F}$ (as in the present volume).

3.6.3.6. Symmetry operations

Listed under the heading of *Symmetry operations* is the geometric description of the symmetry operations of the magnetic group. A symbol denoting the geometric description of each symmetry operation is given. Details of this symbolism, except for the use of prime to denote time inversion, are given in Sections 1.4.2 and 2.1.3.9. For glide planes and screw axes, the glide and screw part are always explicitly given in parentheses by fractional coordinates, *i.e.* by fractions of the basis vectors of the coordinate system of $\mathcal{F}$ of the superfamily of the magnetic group. A coordinate triplet indicating the location and orientation of the symmetry element is given, and for rotation-inversions the location of the inversion point is also given. These symbols, with the addition of a prime to denote time inversion, follow those used in the present volume, *IT* E and Litvin (2005, 2008*b*). In addition, each symmetry operation is also given in Seitz (1934, 1935*a*,*b*, 1936) notation (see Section 3.6.2.2.3), *e.g.* see Table 3.6.3.1 for the symmetry operations of the magnetic space group 51.14.400 $P_{2b}mma'$.

The corresponding coordinate triplets of the *General positions,* see Section 3.6.3.9, may be interpreted as a second description of the symmetry operations, a description in matrix form. The numbering (1), (2), ..., (p), ... of the entries in the blocks *Symmetry operations* is the same as the numbering of the corresponding coordinate triplets of the *General position*, the first block below *Positions*. For all magnetic groups with primitive

Table 3.6.3.2
General positions of magnetic space group 51.14.400 $P_{2b}mma'$

Positions	Coordinates			
	$(0, 0, 0)+$ $(0, 1, 0)'+$			
16 *l* 1	(1) x, y, z $[u, v, w]$	(2) $\overline{x}+1/2, \overline{y}, z$ $[\overline{u}, \overline{v}, w]$	(3) $\overline{x}, y, \overline{z}$ $[u, \overline{v}, w]$	(4) $x+1/2, \overline{y}, \overline{z}$ $[\overline{u}, v, w]$
	(5) $\overline{x}, \overline{y}, \overline{z}$ $[\overline{u}, \overline{v}, \overline{w}]$	(6) $x+1/2, y, \overline{z}$ $[u, v, \overline{w}]$	(7) $x, \overline{y}, z$ $[\overline{u}, v, \overline{w}]$	(8) $\overline{x}+1/2, y, z$ $[u, \overline{v}, \overline{w}]$

lattices, the two lists, *Symmetry operations* and *General position*, have the same number of entries.

For magnetic groups with centred cells, only one block of several (two, three or four) blocks of the general positions is explicitly given, see Table 3.6.3.2. A set of two, three or four centring translations is given below the subheading *Coordinates*. Each of these translations is added to the given block of general positions to obtain the complete set of blocks of general positions. While one of the several blocks of general positions is explicitly given, the corresponding symmetry operations are all explicitly given. Each corresponding block of symmetry operations is listed under a subheading of 'centring translation + set' for each centring translation listed below the subheading *Coordinates*.

3.6.3.7. Abbreviated headline

On the second and subsequent pages of the tables for a specific magnetic group there is an abbreviated headline. This abbreviated headline contains three items: (1) the word 'Continued', (2) the three-part number of the magnetic group type, and (3) the short international (Hermann–Mauguin) symbol for the magnetic group type.

3.6.3.8. Generators selected

The line *Generators selected* lists the symmetry operations selected to generate the symmetry-equivalent points of the *General position* from a point with coordinates x, y, z. The first generator is always the identity operation given by (1) followed by generating translations. Additional generators are given as numbers (p), which refer to the coordinate triplets of the *General position* and to corresponding symmetry operations in the first block, if more than one, of the *Symmetry operations*.

3.6.3.9. General and special positions with spins (magnetic moments)

The entries under *Positions*, referred to as *Wyckoff positions*, consist of the *General position*, the upper block, followed by blocks of *Special positions*. The upper block of positions, the general position, is a set of symmetry-equivalent points where each point is left invariant only by the identity operation or, for magnetic groups $\mathcal{F}1'$, by the identity operation and time inversion, but by no other symmetry operations of the magnetic group. The lower blocks, the special positions, are sets of symmetry-equivalent points where each point is left invariant by at least one additional operation in addition to the identity operation, or, for magnetic space groups $\mathcal{F}1'$, in addition to the identity operation and time inversion.

For each block of positions the following information is provided:

Multiplicity: The multiplicity is the number of equivalent positions in the conventional unit cell of the non-primed group $\mathcal{F}$ associated with the magnetic group.

Wyckoff letter: This letter is a coding scheme for the blocks of positions, starting with '*a*' at the bottom block and continuing upwards in alphabetical order.

Site symmetry: The site-symmetry group is the largest subgroup of the magnetic space group that leaves invariant the first position in each block of positions. This group is isomorphic to a subgroup of the point group of the magnetic group. An 'oriented' symbol is used to show how the symmetry elements at a site are related to the conventional crystallographic basis, and the sequence of characters in the symbol correspond to the sequence of symmetry directions in the magnetic group symbol. Sets of equivalent symmetry directions that do not contribute any element to the site symmetry are represented by dots. Sets of symmetry directions having more than one equivalent direction may require more than one character if the site-symmetry group belongs to a lower crystal system. For example, for the 2*c* position of the magnetic space group $P4'm'm$ (99.3.825) the site-symmetry group is '$2m'm'$.'. The two characters $m'm'$ represent the secondary set of tetragonal symmetry directions, whereas the dot represents the tertiary tetragonal symmetry directions.

Coordinates of positions and components of magnetic moments: In each block of positions, the coordinates of each position are given. Immediately following each set of position coordinates are the components of the symmetry-allowed magnetic moment at that position. The components of the magnetic moment of the first position are determined from the given site-symmetry group. The components of the magnetic moments at the remaining positions are determined by applying the symmetry operations to the components of that magnetic moment at the first position.

3.6.3.10. Symmetry of special projections

The symmetry of special projections is given for the two- and three-dimensional magnetic groups. For each three-dimensional magnetic group, the symmetry is given for three projections, projections onto planes normal to the projection directions. If there are three symmetry directions, the three projection directions correspond to primary, secondary and tertiary symmetry directions. If there are fewer than three symmetry directions, the additional projection direction or directions are taken along coordinate axes. For two-dimensional magnetic groups, there are two orthogonal projections. The projections are onto lines normal to the projection directions.

For the three-dimensional magnetic space groups, each projection gives rise to a two-dimensional magnetic space group. For two-dimensional magnetic space groups, each projection gives rise to a one-dimensional magnetic space group. For magnetic rod groups and magnetic layer groups, a projection along the [001] direction gives rise, respectively, to a two-dimensional magnetic point group and a two-dimensional magnetic space group. All other projections give rise to magnetic frieze groups. For magnetic frieze groups, projections give rise to either a one-dimensional magnetic space group or a one-dimensional magnetic point group. The international (Hermann–Mauguin) symbol of the symmetry group of each projection is given. Below this symbol, the basis vector(s) of the projected symmetry group and the origin of the projected symmetry group are given in terms of the basis vector(s) of the projected magnetic group. The location of the origin of the symmetry group of the

Table 3.6.4.1
Comparisons of three-dimensional OG and BNS magnetic group type symbols

Serial No.	OG	BNS	$\mathcal{F}(\mathcal{D})$
44.1.324	*Imm*2		
44.2.325	*Imm*21′		
44.3.326	*Im*′*m*2′		
44.4.327	*Im*′*m*′2		
44.5.328	$I_P mm2$	$P_I mm2$	*Imm*2(*Pmm*2)
44.6.329	$I_P mm'2'$	$P_I mm2_1$	*Imm*2($Pmm2_1$)
44.7.330	$I_P m'm'2$	$P_I nn2$	*Imm*2(*Pnn*2)

projection is given with respect to the unit cell of the magnetic group from which it has been projected.

3.6.4. Comparison of OG and BNS magnetic group type symbols

There are other notations for magnetic group type symbols than the notations of Opechowski & Guccione (1965) and Belov, Neronova & Smirnova (1957): for example for the three-dimensional magnetic group 55.10.450 $P_{2c}b'a'm$ the Shubnikov notation is $Ш_{58}^{403}$ (Koptsik, 1966; Shubnikov & Koptsik, 1974) or Sh_{58}^{403} (Ozerov, 1969*a*,*b*) (see also Zamorzaev, 1976). There are also the variations of the Opechowski & Guccione notation put forward by Grimmer (2009, 2010). We shall limit ourselves here to a detailed comparison of the Opechowski & Guccione and Belov, Neronova & Smirnova notations.

For all group types in the reduced magnetic superfamily of $\mathcal{F}$, the Opechowski & Guccione (1965) magnetic group type symbols (OG symbols) are based on the symbol of the group $\mathcal{F}$. Belov, Neronova & Smirnova (1957) also base their symbols (BNS symbols) on the symbol of the group $\mathcal{F}$, but only for magnetic groups of the type $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$. For magnetic groups $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup (\mathcal{F} - \mathcal{D})1'$, where $\mathcal{D}$ is an equi-class subgroup of $\mathcal{F}$, the BNS symbol is based on the symbol of the group $\mathcal{D}$, the non-primed subgroup of index 2. A magnetic group $\mathcal{M}_R$ can be written as $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha'\mathcal{D}$, where t_α is a translation of $\mathcal{F}$ not in $\mathcal{D}$. The BNS symbol for a magnetic group of the type $\mathcal{M}_R$ is the symbol for the group type $\mathcal{D}$ with a subindex inserted on the symbol for the translational subgroup of $\mathcal{D}$ to denote the translation t_α'.

Example

The representative three-dimensional space group $\mathcal{F} = Pmm2$ has a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 1\}$ and the standard set of coset representatives

$$\{1|0\} \quad \{m_{100}|0\} \quad \{m_{010}|0\} \quad \{2_{001}|0\}.$$

The three-dimensional magnetic space group 25.10.165 $\mathcal{F}(\mathcal{D}) = Pmm2(Pcc2)$ has a subgroup $\mathcal{D}$ with a translational subgroup generated by the three translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$, $t_\alpha' = \{1|0, 0, 1\}'$, and a set of coset representatives

$$\{1|0\} \quad \{m_{100}|0, 0, 1\} \quad \{m_{010}|0, 0, 1\} \quad \{2_{001}|0\}.$$

The OG magnetic group type symbol is, see Section 3.6.2.2.4, $P_{2c}m'm'2$, *i.e.* based on the symbol for the group type $\mathcal{F} = Pmm2$. The BNS symbol is $P_c cc2$, *i.e.* based on the symbol for the subgroup $\mathcal{D} = Pcc2$ of $\mathcal{F}$, with a subindex '*c*' attached to '*P*' to denote the translation $t_\alpha' = \{1|0, 0, 1\}'$ in $\mathcal{M}_R = \mathcal{F}(\mathcal{D}) = \mathcal{D} \cup t_\alpha'\mathcal{D}$.

A side-by-side comparison of OG magnetic group type symbols and BNS symbols is given in Litvin (2013). As the OG and BNS symbols are the same for magnetic groups $\mathcal{F}$, $\mathcal{F}1'$ and $\mathcal{M}_T$, BNS symbols are explicitly listed only for groups of type $\mathcal{M}_R$. Examples of this comparison are given in Table 3.6.4.1.

3.6.5. Maximal subgroups of index ≤ 4

We consider the maximal subgroups of index ≤ 4 of the one-, two- and three-dimensional magnetic space groups and the two- and three-dimensional magnetic subperiodic groups. A complete listing of the maximal subgroups of the two- and three-dimensional non-primed space groups can be found in *International Tables for Crystallography*, Volume A1, *Symmetry Relations Between Space Groups* (2010; *IT* A1). The maximal subgroups of index ≤ 4 of the three-dimensional non-primed space groups and non-primed layer and rod groups can also be found on the Bilbao Crystallographic Server (http://www.cryst.ehu.es; Aroyo *et al*., 2006).

For magnetic groups, an abstract of a method for determining the maximal subgroups of magnetic groups was published by Sayari & Billiet (1977). The maximal subgroups of magnetic groups found in Litvin (2013) were derived from Litvin (2008*a*) using a method given by Litvin (1996).

Each maximal subgroup table is headed by the magnetic group type whose maximal subgroup types are to be listed.

Examples

For the three-dimensional magnetic space group type $Pb'a'm$, one finds (Litvin, 2013), in bold blue type, information which defines the representative group of this type in a coordinate system O; **a**, **b**, **c**:

55.5.445 $Pb'a'm$ (0, 0, 0; **a**, **b**, **c**)

$\{1\|0\}$	$\{2_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}'$
$\{2_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{2_{001}\|0\}$
$\{\overline{1}\|0\}$	$\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}'$
$\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{m_{001}\|0\}$

The first column gives the global serial number of the group, followed in the second column by its magnetic group type symbol. In the third column, the symbol (O; **a**′, **b**′, **c**′) gives the origin O and basis vectors **a**′, **b**′, **c**′ of the conventional unit cell of the non-primed subgroup of the representative group of the type $Pb'a'm$. These basis vectors **a**′, **b**′, **c**′ imply both the magnetic and non-primed translational subgroups of the representative group. In this case, the P translational subgroup of the representative group is non-primed and generated by the basis vectors **a**, **b**, **c**. The standard set of coset representatives of this representative group is given on the right.

For the three-dimensional magnetic space-group type $P_{2b}ma2$ one finds (Litvin, 2013):

28.6.190 $P_{2b}ma2$ (0, 0, 0; **a**, 2**b**, **c**)

$\{1\|0\}$	$\{m_{100}\|\frac{1}{2}, 0, 0\}$
$\{m_{010}\|\frac{1}{2}, 0, 0\}$	$\{2_{001}\|0\}$

Note here that **a**′ = **a**, **b**′ = 2**b**, **c**′ = **c**, being the basis vectors of the conventional unit cell of the non-primed subgroup of the representative group of $P_{2b}ma2$, implies that the translational subgroup of the representative group is P_{2b}, *i.e.* generated by the non-primed translations $\{1|1, 0, 0\}$, $\{1|0, 2, 0\}$, $\{1|0, 0, 1\}$ and the magnetic translation $\{1|0, 1, 0\}'$.

Following the subtable heading of each magnetic space-group type is a listing of the maximal subgroups of index ≤ 4 of the representative magnetic space group of this type.

Examples

From the list of maximal subgroups of the representative magnetic group of the type $Pb'a'm$ is the subgroup listed as

$Pb'a'2$	2	$(0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c})$	$\{1\|0\}$	$\{2_{001}\|0\}$
			$\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}'$

The first column gives the magnetic group type symbol of the subgroup. The second column gives the subgroup index of this subgroup as a subgroup of the representative group of type $Pb'a'm$. In the third column, the symbol $(O + \mathbf{p}; \mathbf{a}', \mathbf{b}', \mathbf{c}')$ gives the origin '$O + \mathbf{p}$' and basis vectors $\mathbf{a}'$, $\mathbf{b}'$, $\mathbf{c}'$ of the conventional unit cell of the non-primed subgroup, where $\mathbf{p}$, a translation of the origin of the coordinate system of the representative group $Pb'a'm$, and the conventional unit cell are such that the coset representatives listed are transformed into the standard cosets of the representative group of the subgroup type $Pb'a'2$. In this case, since the listed coset representatives are the standard cosets of the representative group of type $Pb'a'2$, no translation of origin is required, and consequently $O + \mathbf{p} = 0, 0, 0$. The conventional unit cell of the non-primed subgroup of the subgroup $Pb'a'2$ is the same as that of representative group of the type $Pb'a'2$ and consequently one finds $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$.

That the listed coset representatives of the subgroup are the same as those of the representative group of that subgroup type is not always the case:

Example

A subgroup of type $P2/m$ of the representative group $Pb'a'm$ is listed as

$P2/m$	2	$(0, 0, 0; \mathbf{b}, \mathbf{c}, \mathbf{a})$	$\{1\|0\}$	$\{2_{001}\|0\}$	$\{\bar{1}\|0\}$	$\{m_{001}\|0\}$

The standard set of coset representatives of the representative group $P2/m$ are

$$\{1|0\} \quad \{\bar{1}|0\} \quad \{2_{010}|0\} \quad \{m_{010}|0\}.$$

A change in setting to have the coset representatives of the subgroup be identical with the coset representatives of the representative group $P2/m$ is represented in the symbol $(0, 0, 0; \mathbf{b}, \mathbf{c}, \mathbf{a})$, *i.e.* changing the setting from $\mathbf{a}, \mathbf{b}, \mathbf{c}$ to $\mathbf{b}, \mathbf{c}, \mathbf{a}$.

Other cases may require a simultaneous change to both the origin and the setting of the conventional unit cell of the non-primed subgroup:

Example

A third subgroup of the representative group $Pb'a'm$ is the equi-class subgroup of the same type $Pb'a'm$:

$Pb'a'm$	2	$(0, 0, \frac{1}{2}; \mathbf{a}, \mathbf{b}, 2\mathbf{c})$	$\{1\|0\}$	$\{2_{100}\|\frac{1}{2}, \frac{1}{2}, 1\}'$
			$\{2_{010}\|\frac{1}{2}, \frac{1}{2}, 1\}'$	$\{2_{001}\|0\}$
			$\{\bar{1}\|0, 0, 1\}$	$\{m_{100}\|\frac{1}{2}, \frac{1}{2}, 0\}'$
			$\{m_{010}\|\frac{1}{2}, \frac{1}{2}, 0\}'$	$\{m_{001}\|0, 0, 1\}$

The listed coset representatives of this subgroup are not the same as the coset representatives of the representative group $Pb'a'm$, *i.e.* where the z component of the non-primitive translation associated with all coset representatives is zero. To have these listed coset representatives become identical with the coset representatives of the standard representative group of $Pb'a'm$, one must change the origin of the coordinate system. This information is provided in the symbol $(0, 0, \frac{1}{2}; \mathbf{a}, \mathbf{b}, 2\mathbf{c})$ where $O + \mathbf{p} = 0, 0, \frac{1}{2}$ denotes the translation under which all the non-zero z components of the coset representatives are transformed to zero. Note also that the P in the subgroup symbol denotes a non-primed translational subgroup which is determined by $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *i.e.* P denotes the translational group generated by the translations $\{1|1, 0, 0\}$, $\{1|0, 1, 0\}$ and $\{1|0, 0, 2\}$.

In the tabulations of the maximal subgroups of groups of the type $\mathcal{F}1'$ not all maximal subgroups are explicitly listed. The maximal subgroup $\mathcal{F}$ of $\mathcal{F}1'$ is not listed. If $\mathcal{G}$ is a maximal subgroup of $\mathcal{F}$, then $\mathcal{G}1'$ is a maximal subgroup of $\mathcal{F}1'$ and is also not explicitly listed. All maximal subgroups $\mathcal{G}$ of $\mathcal{F}$ are listed under $\mathcal{F}$, and consequently, all maximal subgroups $\mathcal{G}1'$ of $\mathcal{F}1'$ are then found from the list of all maximal subgroups $\mathcal{G}$ of $\mathcal{F}$ by multiplying each by $1'$. For each listed maximal subgroup, its non-primed subgroup type is explicitly given. For example, a listed subgroup of $Pma21'$ is

$Pma'2'$	Pm	2	$(0, 0, 0; \mathbf{a}, \mathbf{b}, \mathbf{c})$	$\{1\|0\}$	$\{2_{001}\|0\}'$
				$\{m_{010}\|\frac{1}{2}, 0, 0\}'$	$\{m_{100}\|\frac{1}{2}, 0, 0\}$

where the non-primed subgroup type Pm of $Pma'2'$ is given in the second column.

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